



METER

LABROS

SOILVIEW-ANALYSIS FOR VARIOS

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1. INTRODUCTION

Thank you for choosing the VARIOS automated measurement and evaluation system for determining thermal conductivity of soil samples from METER Group.

This user manual covers the operation of the LABROS SoilView-Analysis software, used to evaluate measurements obtained using the Transient Line Heat Source Method in the VARIOS. Read the VARIOS User Manual along with this manual. Both are available on the [VARIOS support](https://meter.ly/varios-support) page (meter.ly/varios-support). Scientific background related to determining thermal conductivity of soil samples is provided in both manuals.

LABROS SoilView-Analysis software is available for download also at the [VARIOS support](https://meter.ly/varios-support) page (<https://meter.ly/varios-support>).

LABROS SoilView-Analysis is compatible with Microsoft® Windows® 10 or newer. The software reads data recorded in VARIOS projects by the data acquisition software LABROS SoilView and stored as *.var ios files.

LABROS SoilView-Analysis performs the following operations:

- Applies required parameters for evaluating recorded experimental data such as column length and tare weights of the measurement device components.
- Visualizes the raw data for thermal conductivity values and weight changes.
- Recalculates thermal conductivity values and net weight data to find volumetric water content.
- Calculates and visualizes the data for thermal conductivity characteristics.
- Applies state-of-the-art thermal fitting models to the data, visualizes functions, and lists of the values and confidence limits of the conductivity parameters.
- Exports graphs, raw data, calculated data, fitted functions, and other parameters of interest.

VARIOS combines a simple evaporation method with the measurement of thermal conductivities via the single-needle probe. Actual volumetric water contents (VWC), $\theta \text{ m}^3/\text{m}^3$, are derived by continuously recording sample weights during the drying process caused by evaporation. Thermal conductivity of the soil column, $\lambda \text{ Wm}^{-1}\text{K}^{-1}$, is measured via the single needle probe in high-temporal resolution. Therefore, VARIOS yields high-resolution measurements of the VWC to thermal conductivity, $\lambda(\theta)$, relationship. The basic principle and the scientific background of this combination is outlined in Markert et al. (2016).

2. OPERATION

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

2.1 INSTALLATION

Use the instructions in this section to install the LABROS SoilView-Analysis software on a laptop or personal computer running Microsoft Windows 10 or newer operating system.

NOTE: The LABROS SoilView-Analysis software is only compatible with Microsoft Windows 10 or newer. It will not run on a laptop running an iOS operating system (Mac).

1. Navigate to the METER VARIOS Support webpage (<https://meter.ly/varios-support>).
2. Click on the LABROS SoilView and LABROS SoilView-Analysis software download link. The LABROSSoilView_vx.x.x.exe file will be downloaded to the computer Downloads folder.
3. Double click on the LABROSSoilView_vx.x.x.exe file to start the installation.

NOTE: If there is a problem executing the LABROSSoilView_vx.x.x.exe file, please download and install Microsoft .NET Framework 4.8 manually and be sure to have the current version of the Windows installer.
4. Click on the **Next** button in the lower-right corner of the LABROSSoilView 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 only LABROS SoilView-Analysis do the following (Figure 1):
 - i. Click on the Down Arrow next to the software that should NOT be installed.
 - ii. Select the **Entire feature will be unavailable** option from the dropdown list that appears.
 - iii. Click on the **Next** button to start the installation.

This will keep the selected feature from being installed.
5. Follow the instructions in the installation wizard window until installation is complete.

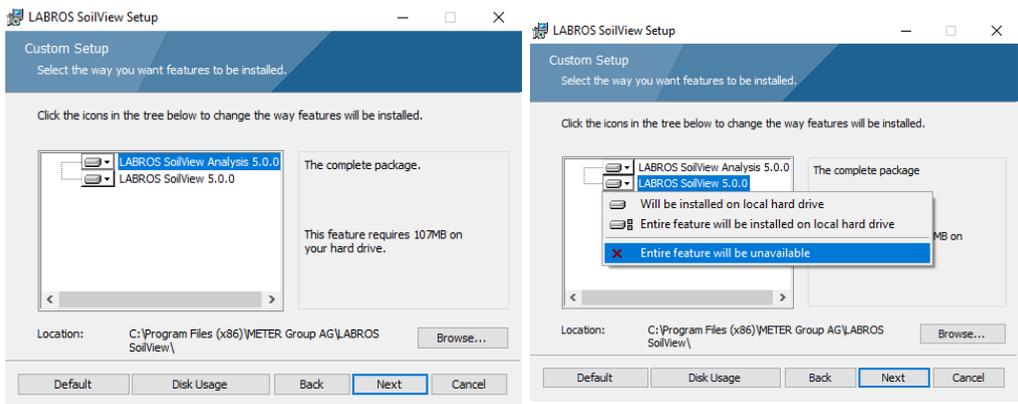


Figure 1 Custom Setup screens

2.2 USER MODES

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

2.2.1 PUBLIC USER MODE

In Public User mode the software runs with default values applied to most specifications (e.g., soil surface area or weight corrections).

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 tab (**Information, Measurement, Evaluation, Fitting, or Export**). The change will be active immediately.

2.2.2 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 for data processing. Power User mode allows the user to alter many of the default values or manipulate measurement data.

POWER USER MODE EXAMPLES

- Measurement data records that are obvious outliers can be edited or deleted, or undesired records can be deleted at the beginning or end of a measurement campaign.
- Data that are measured on different devices (e.g., for experiments with different soil column heights) can be processed.

IMPORTANT: Changed parameters will affect the results of the data processing and the implications on the calculations must be known by the users (the software will not compensate automatically). The Power User mode is available for those that know soil physics well. The Power User mode is not recommended for all other users.

2.3 STARTING THE PROGRAM

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

1. Open the Windows Start menu.
2. Select LABROS SoilView-Analysis (or LABROS SoilView) from the list of programs.

On the first start of the software a welcome screen will appear. The welcome window shows the LABROS software and file location, and two toolbar lines ([Figure 2](#)).

The first toolbar below the LABROS software and file location contains the **File, Extra,** and **Help** drop-down menus.

The second toolbar contains icons for **Show file explorer, Open, Save, Save as, Feedback, Settings,** and **Manual**.

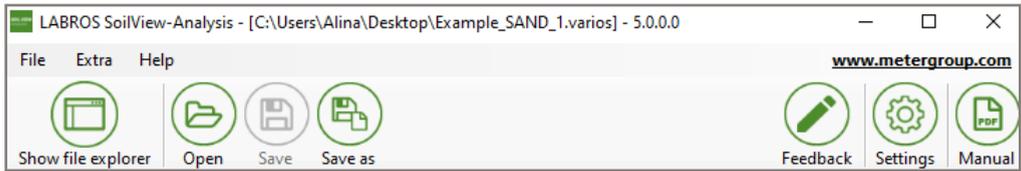


Figure 2 Welcome screen

NOTE: The Feedback icon can be used for sending feature requests, bug reports, questions, or other comments. Please be sure to enter a correct email address.

For more information about updates the user can do one of the following to view a PDF file:

- In the **What is new in Version** pop-up window that appears when software first starts up, select the two arrow icon (>>) at the end of each item to open a PDF with more detail (Figure 3).

NOTE: If you select Don't show me this again when the What is new in version window pops up, this option will no longer be available.

- Select the **Help** menu item on the first toolbar and then **What is New** from the dropdown list.

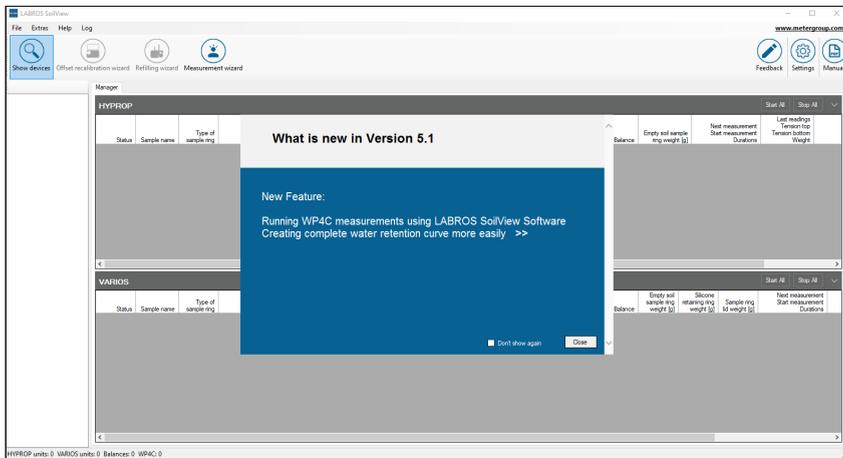


Figure 3 What is new pop-up window

If data sets were loaded in the previous session, LABROS SoilView-Analysis will automatically load the data set last used. 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 datasets will have to be reloaded.

3. PROCESSING VARIOS PROJECTS

The information in this section describes the software menus and how to set up VARIOS projects in the LABROS SoilView-Analysis software.

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

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

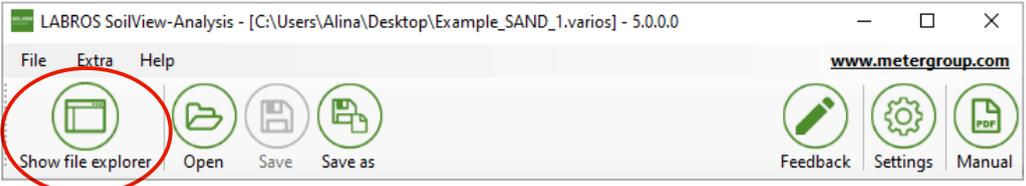


Figure 4 Show/Hide toggle command

The **Save** icon opens a Save window enabling the user to name the file and choose where the file will be saved. When command icons or entries are shown in gray they cannot be used. For example, the **Save** icon can only be used if a project has been opened and modified (Figure 5).

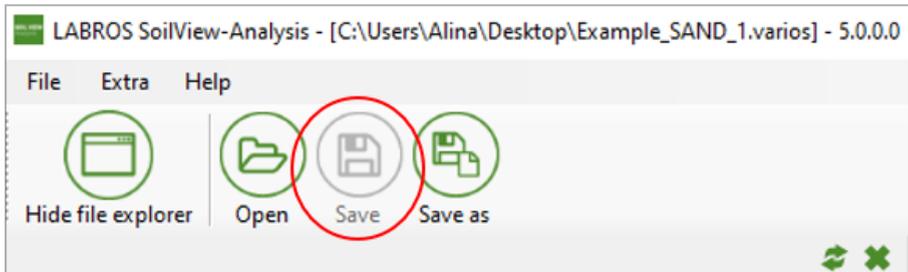


Figure 5 Save/Save as command

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

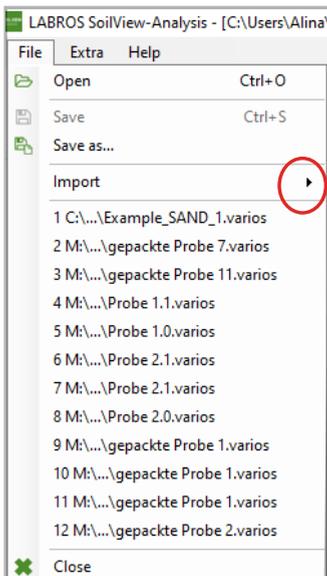


Figure 6 List of additional command actions

Entries can sometimes be selected by key-combinations or shortcuts. If available the combinations are indicated to the right of the respective entry.

To return to a previous menu or action press the **ESC** button.

Data from VARIOS project files (*.varios) can be processed in the LABROS SoilView-Analysis software.

3.1 OPENING A PROJECT FILE

The **File** menu is used to open and save project files.

With an existing data file, follow the instructions below to open the project.

1. Select **File** from the toolbar menu (Figure 7).

LABROS SOILVIEW-ANALYSIS FOR VARIOS

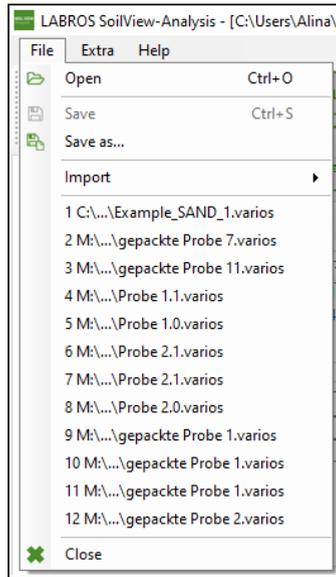


Figure 7 Select File menu

2. Select **Open** from the dropdown list (Figure 7).
The Open window will appear (Figure 8).

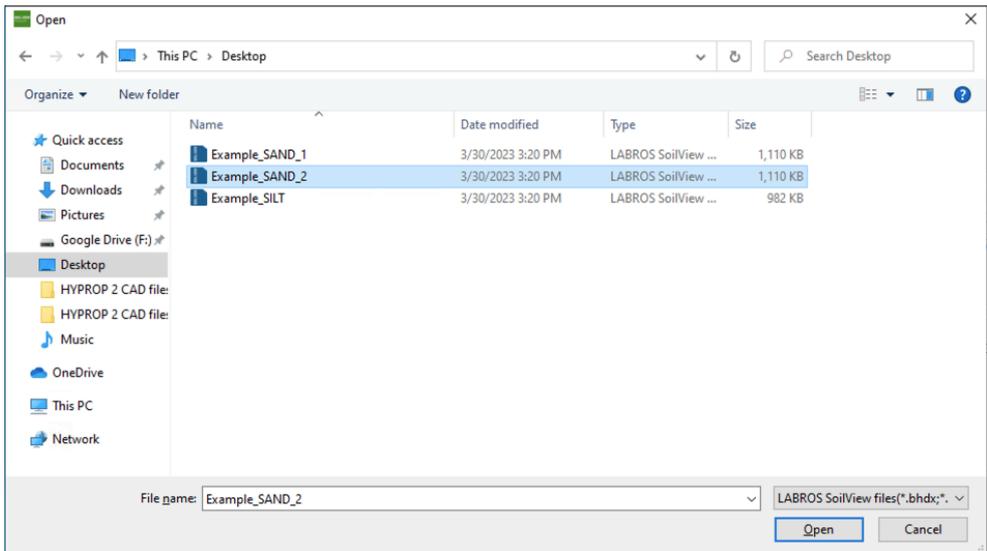


Figure 8 File > Open window

3. Select the desired file by navigating in the Open window to the appropriate folder (Figure 8).

Only files with LABROS SoilView-Analysis compatible extensions will show in the Open window.

4. 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).

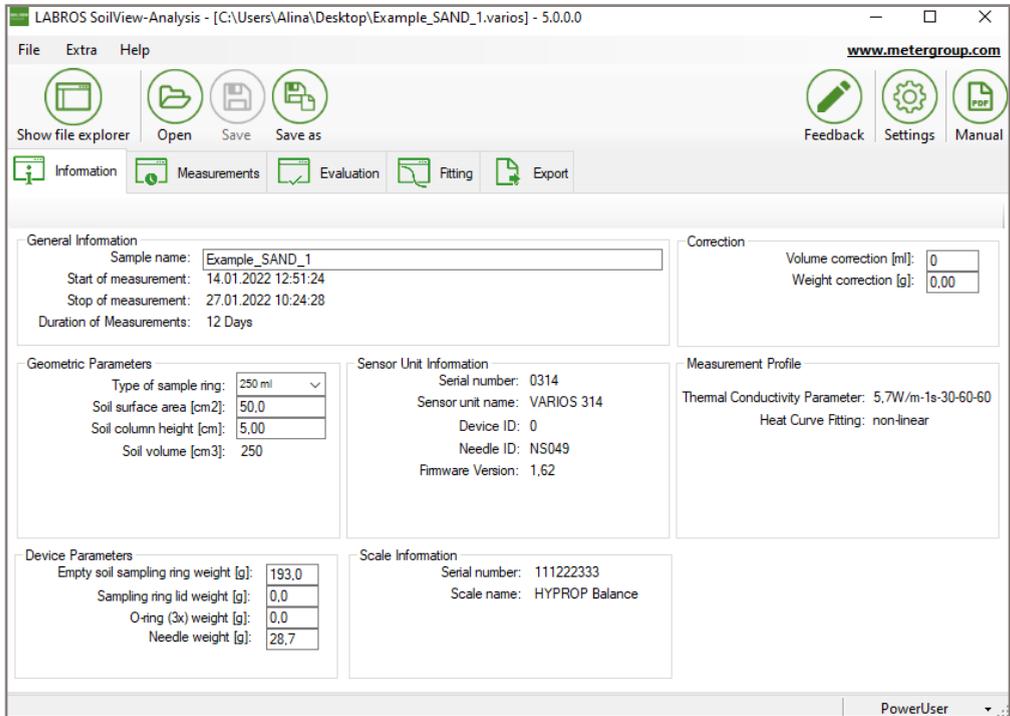


Figure 9 Open window

3.2 FILE MENU OPTION DEFINITIONS

The following subsections describe the **File** menu options and definitions.

3.2.1 FILE > OPEN

The **File > Open** option is the first entry in the **File** menu. Table 1 describes the type of data file that can be opened.

Table 1 Data File Type Description

File Type	Descriptions
*.varios (default)	A LABROS SoilView-Analysis version 5.0 (or higher) project file containing information, measurement data, calculated thermal conductivity data, and fitted function for a single measurement campaign.

NOTE: Measurement files are not backward compatible.

3.2.2 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 and **Save** menu entry will be gray to indicate it is inactive.

3.2.3 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 during the data acquisition stage. However, this original file is write-protected as long as the measurement campaign continues. If preferred the file can be saved with a different name.

3.2.4 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 project files by selecting the project filename.

3.2.5 FILE > CLOSE

The **Close** option closes the data file. If changes have been made a message window asking for confirmation to save changes will appear.

3.3 HELP MENU

The **Help** menu contains LABROS SoilView-Analysis information for the user. The following subsections describe options provided in the **Help** menu (Figure 10).

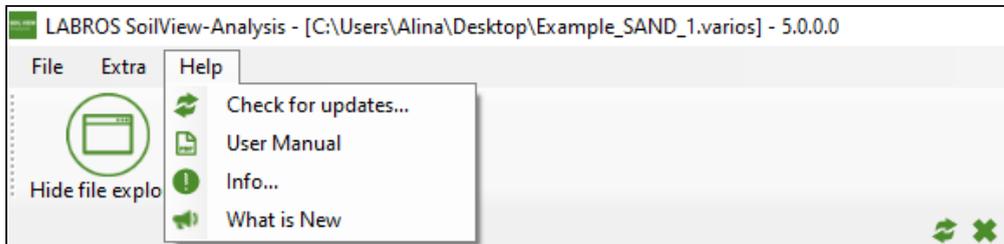


Figure 10 Help menu

3.3.1 CHECK FOR UPDATES

The **Check for updates...** option gives information about new available software versions and provides a download link if necessary.

3.3.2 USER MANUAL

The **User Manual** option provides the current version of LABROS SoilView-Analysis User Manual as a PDF document for viewing, printing, or downloading.

3.3.3 INFO...

The **Info...** option shows the LABROS SoilView-Analysis software version in use, lists the VARIOS development team, and shows the disclaimer.

3.3.4 WHAT IS NEW

The **What is New** option shows a PDF file describing all new features and bug fixes that apply to the current version of the LABROS SoilView-Analysis software.

4. REGISTERS FOR PROCESSING DATA

The LABROS SoilView-Analysis software groups data processing in five registers (Figure 11) for VARIOS dryout measurement, and VARIOS standalone:

- Information Register
- Measurements Register
- Evaluation Register (dryout measurement only)
- Fitting Register (dryout measurement only)
- Export Registers

Only three register groups in the LABROS SoilView-Analysis software are available for the VARIOS standalone:

- Information Register
- Measurements Register
- Export Registers

The registers include all steps of the data evaluation process in a logical, consecutive sequence. Normally the register tabs are used from left to right. Data processing options can be specified and data can be edited or manipulated in all register tabs by selecting the Power User mode.



Figure 11 Register groups

Uses, actions, and edits that are available in all registers:

- Values that can be edited are shown in an edit field.
- Values that cannot be modified are shown without the edit field.
- All variables that are expressed by numerical values are given with units (metric or imperial). If a user edits a numerical value, the new value must be in the same unit.
- Whether or not a variable can be edited depends on which user mode is used. Power Users can edit more fields than Public Users (Section 2.2).
- When inserting a numerical value, the proper decimal separator sign depends on the region settings of the computer. Default decimal separator for the German Operating System is the comma, and the default decimal separator for the English Operating System is a period.
- Fields for numerical values do not accept alphabetical letters or special characters. If a user attempts to insert a character that is not permitted the field does not show the typed character.

- To save an input operation the cursor must leave the input field in one of the following ways:
 - ◆ Press the keyboard **Tab** key
 - ◆ Press the keyboard **Enter/Return** key
 - ◆ Move the cursor with the mouse to another position in the window and left-click the mouse.

In some menus an **Accept** button will appear and must be pressed.

- Hovering the cursor over an icon or register tab will show a pop-up with information (Quickinfo) about the function for 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.

4.1 INFORMATION REGISTER

This section describes how to use the **Information** register tab (Figure 12) to specify the required parameters for the measurement.

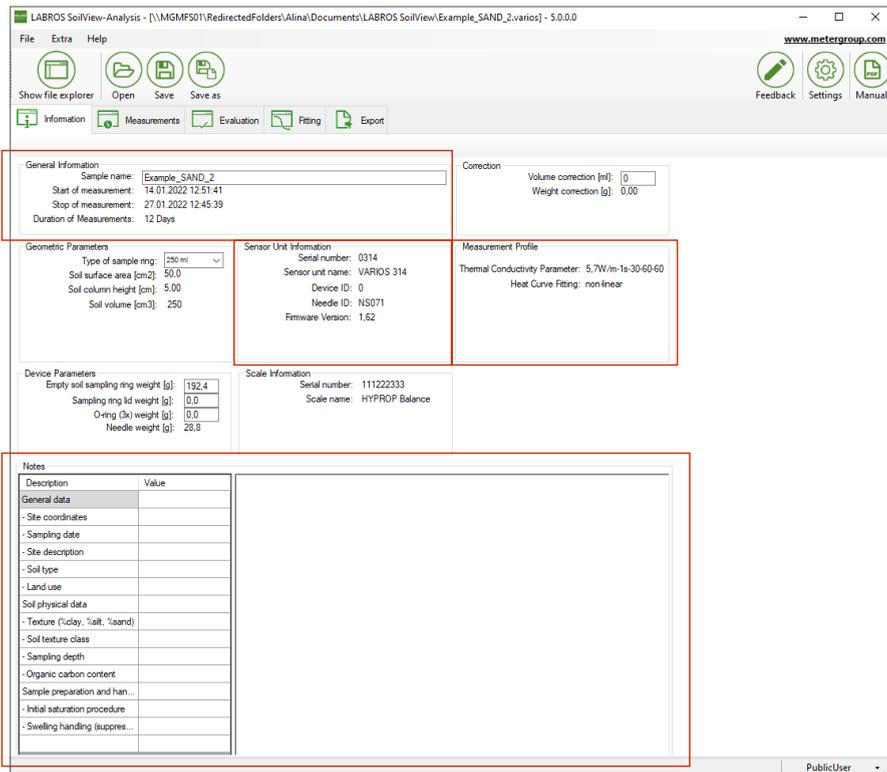


Figure 12 Information register

The **Information** register is the first of five register tabs (Figure 12). When the **Information** tab is selected it displays a window that contains eight blocks or subcategories (used for the VARIOS dryout measurement), or four blocks (used for the VARIOS Standalone measurement) providing an overview of the selected project. The four blocks used for the VARIOS Standalone method are outlined in red (Figure 12).

4.2 DATA GROUPS

The following sections show examples of the different data groups accessed on the **Information** register. Tables with definitions and editing options for each data group are also provided below.

4.2.1 GENERAL INFORMATION

General Information

Sample name:

Start of measurement: 14.01.2022 12:51:24

Stop of measurement: 27.01.2022 10:24:28

Duration of Measurements: 12 Days

Figure 13 General Information

Table 2 Data Group General Information

Variable	Explanation	Data Value	Editable	
			Public User	Power User
Sample name	The name can be chosen by the user. NOTE: By default the sample name is also used for the file name during export. The file name rules, specified by Windows, also have to be considered. If data was captured from a VARIOS 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 recorded in the *.varios file automatically.	–	No	No
Stop of measurement	Date and time from the end of the recorded data. These data are recorded in the *.varios file automatically.	–	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

4.2.1.1 CORRECTION DATA GROUP (DRYOUT MEASUREMENT ONLY)

Correction

Volume correction [ml]:

Weight correction [g]:

Figure 14 Correction

Table 3 Data Group Correction

Variable	Explanation	Data Value	Editable	
			Public User	Power User
Volume correction	Volume correct of the sample is possible and sometimes necessary when sample preparation has errors, deficits, or shows roughness. Correcting the volume will affect the water content calculation because weight changes are related to the sample volume.	0 cm ³	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. This could be the constant weight of 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 for accurate weight correction.	0 g	No	Yes

4.2.1.2 GEOMETRIC PARAMETERS (DRYOUT MEASUREMENT ONLY)

Geometric Parameters

Type of sample ring: ▼

Soil surface area [cm2]:

Soil column height [cm]:

Soil volume [cm3]:

Figure 15 Geometric Parameters

Table 4 Data Group Geometric Parameters

Variable	Explanation	Data Value	Editable	
			Public User	Power User
Type of sample ring	The standard sample ring is the 250 mL ring (standard METER soil sample ring) with two boreholes. If the user already chose the type of sample ring used in the LABROS SoilView software, the selected value is adopted in SoilView-Analysis.	250 ml	Yes	Yes
	A customized sample ring can also be chosen.			
	Geometric parameters have to be adjusted.			
	Selecting a customized sample ring will affect the subsequent default entries for surface area and height.			
	NOTE: The height ratio between the borehole for the needle sensor and the bottom of the sample, as well as the distance of the sensor to the sampling ring must be the same for the METER standard sampling ring (250 ml).			
Soil Surface Area	Shows the surface area of the sample, dependent upon the chosen type of sample ring.	50 cm ²	No	Yes
Soil Column Height	Height of soil sample.	5 cm	No	Yes
	Default value is uses the height of METER standard soil sample rings.			
	Example: If swelling occurred during saturation and the user decided not to cut the saturated sample to exactly 5.0 cm, the Soil Column Height value has to be adjusted.			
Soil Volume	Volume of soil sample is calculated from the entries of area and height.	250 cm ³	No	No

4.2.2 SENSOR UNIT INFORMATION

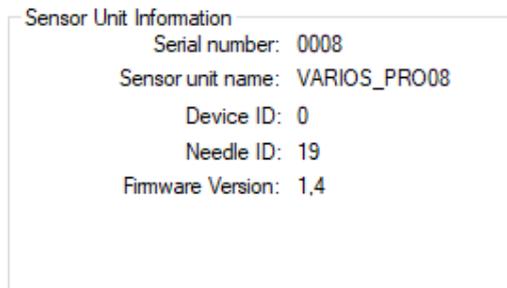


Figure 16 Sensor Unit Information

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

Variable	Explanation	Editable		
		Data Value	Public User	Power User
Serial number	Serial number information for METER firmware provided through *.var ios file. NOTE: This number is always a unique identification of the measurement device. Together with the date information it is a unique identifier of the measurement.	-	No	No
Sensor unit name	Information as specified in data acquisition and stored in the *.var ios file.	-	No	No
Devide ID	Information as specified in data acquisition and stored in the *.var ios file.	-	No	No
Needle ID	Information as specified in data acquisition and stored in the *.var ios file.	-	No	No
Firmware Version	Information given by METER firmware.	-	No	No

4.2.3 MEASUREMENT PROFILE

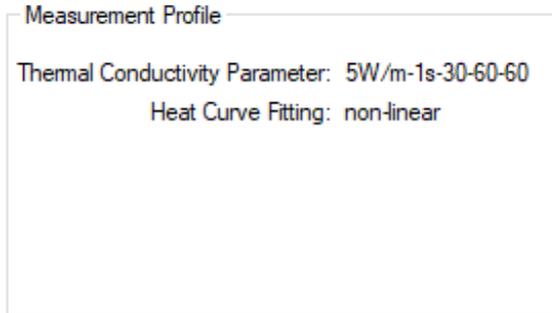


Figure 17 Measurement Profile

Table 6 Data Group Measurement Profile

Variable	Explanation	Editable		
		Data Value	Public User	Power User
Thermal Conductivity Parameter	Shows the measurement parameters defined in the VARIOS Profile settings of the LABROS SoilView data acquisition software.	-	No	No
	Heating power			
	Sampling interval			
	Number of drift samples			
	Number of heat samples			
Heat Curve Fitting	Number of cool samples			
	Shows the used fitting method defined in the LABROS SoilView data acquisition software.	-	No	No
	Nonlinear fitting assumes a nonlinear heating over $\log(t)$ and linear heating over $\log(t-t_0)$. This is the recommended fitting method.			
	Linear fitting assumes a linear heating over $\log(t)$. This fitting method is recommended only for ASTM and IEEE conformity.			

NOTE: For more information about the parameters definition please refer to the Measurement Profile section in the [VARIOS User Manual](http://meter.ly/varios-support) (meter.ly/varios-support).

4.2.3.1 DEVICE PARAMETERS (DRYOUT MEASUREMENT ONLY)

Device Parameters	
Empty soil sampling ring weight [g]:	193,0
Sampling ring lid weight [g]:	16,5
O-ring (3x) weight [g]:	1,66
Needle weight [g]:	28,7

Figure 18 Device Parameters

Table 7 Data Group Device Parameters

Variable	Explanation	Editable		
		Data Value	Public User	Power User
Empty soil sampling ring weight [g]	Exact mass of the soil sampling ring (dry and clean).	-	Yes	Yes
	<p>NOTE: This value must be specified individually for each measurement!</p> <p>The mass can be determined before or after the VARIOS 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%.</p>			
Sample ring lid weight [g]	Exact mass of the sampling ring lid weight (dry and clean).	-	Yes	Yes
	<p>NOTE: This value must be specified individually for each measurement!</p> <p>The mass can be determined before or after the VARIOS measurement. Wrong values transfer linearly to wrong calculated total water contents.</p>			
Silicone retaining ring weight [g]	Exact mass of the o-rings (dry and clean).	-	Yes	Yes
	<p>NOTE: This value must be specified individually for each measurement!</p> <p>The mass can be determined before or after the VARIOS measurement. Wrong values transfer linearly to wrong calculated total water contents.</p>			
Needle weight [g]	Exact mass of the needle sensor (dry and clean).	-	Yes	Yes
	<p>NOTE: This value is individual for each needle sensor.</p> <p>The mass of the needle sensor is stored and automatically transferred from LABROS SoilView data acquisition software.</p>			

4.2.4 SCALE INFORMATION (DRYOUT MEASUREMENT ONLY)

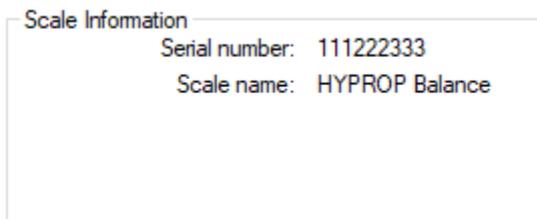


Figure 19 Scale Information

Table 8 Data Group Scale Information

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

4.2.4.1 NOTES

Notes	
Description	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 han...	
- Initial saturation procedure	
- Swelling handling (suppres...	

Figure 20 Notes data group

Table 9 Data Group Notes

Variable	Explanation	Data Value	Editable	
			Public User	Power User
Description	Any information in tabular view.	–	Yes	Yes
	Default value: <ul style="list-style-type: none"> • General data • Site coordinates • Sampling date • Site description • Soil type • Land use 			
	Soil physical data: <ul style="list-style-type: none"> • Texture (%clay, %silt, %sand) • Soil texture class • Sampling depth • Organic carbon content Sample preparation and handling: <ul style="list-style-type: none"> • 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 related to the measurement campaign.	–	Yes	Yes

4.3 MEASUREMENTS REGISTER

This section describes how to use the **Measurements** register tab (Figure 21) for visualization and measured data editing.

The **Measurements** register tab (Figure 21) shows the readings of the needle sensor and the recorded weights when data collection used the dryout measurement setup. The register is composed of four windows for dryout measurement and two windows for standalone measurement.

- The left windows show graphs of the recorded data.
- The right windows show the numerical values.

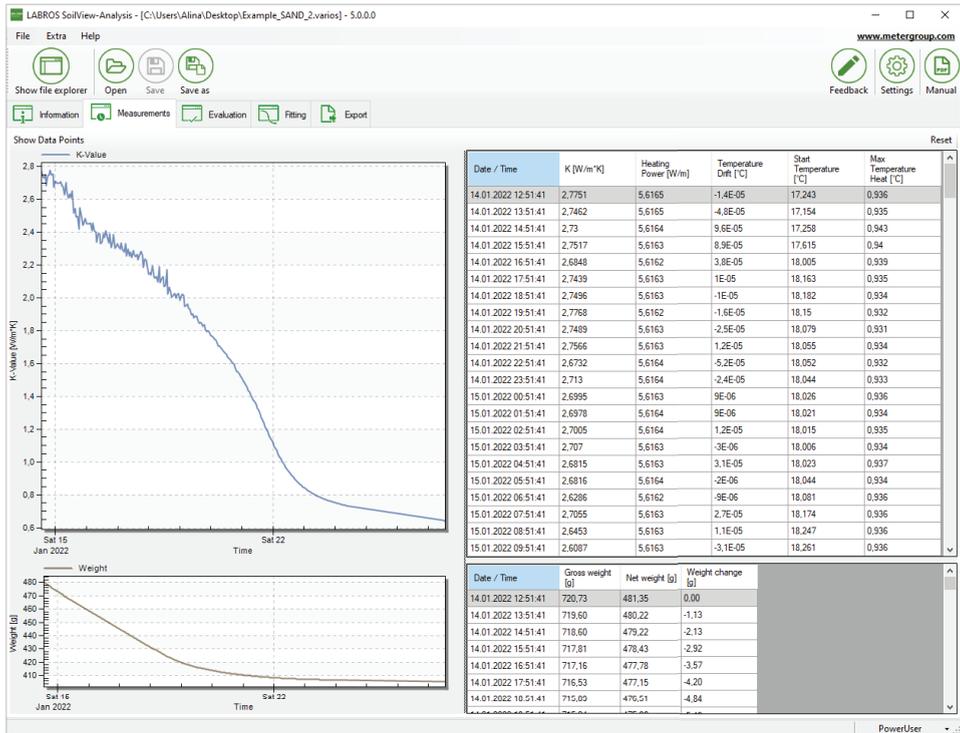


Figure 21 Measurement register (dryout measurement setup)

The size of the data or graph windows can be resized in several ways:

- Place the mouse on a border (invisible) of an individual window and drag the border to a new position.
- When the mouse is directly on a border it changes from a single arrow to a double arrow.
- Each of the graphics windows can be enlarged to full-screen by positioning the mouse on the window, right-clicking the mouse button, and selecting the **Maximize** option in the pop-up menu.
- To leave the full-screen mode press 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 dragging the cursor to the opposite point of a rectangle while holding down the left mouse button (Figure 22).

To reset the window ranges right-click the mouse button and select the **Undo Zoom** option.

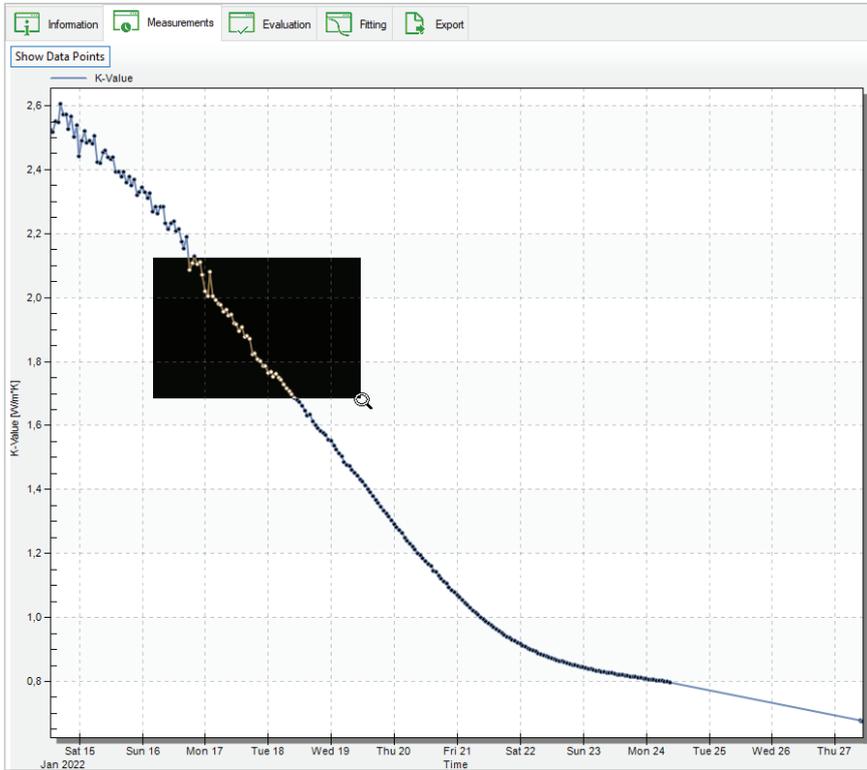


Figure 22 Conductivity graph

4.3.1 INTERPRETATION OF THE CONDUCTIVITY DATA

Figure 22 shows a continuous decrease of both thermal conductivity (top) and sample mass (bottom) during the measurement campaign. This means a decrease in VWC is accompanied by a decrease in thermal conductivity. In the beginning of the measurements the conductivity data show a larger uncertainty (higher fluctuations), whereas at the end of the measurement the curves are very smooth.

This phenomenon occurs because the heating power remained constant and the water content was high in the beginning. Consequently, the thermal conductivity was also high in the beginning. Therefore, the increase in temperature (ΔT) due to the heating was low, which leads to higher uncertainties in the slope of $\Delta T(\ln(t))$. This is reflected in higher uncertainties in the resulting thermal conductivity. At the end of the measurement the thermal conductivity is low leading to higher ΔT . Higher ΔT means lower uncertainties.

4.3.2 DATA VISUALIZATION OPTIONS

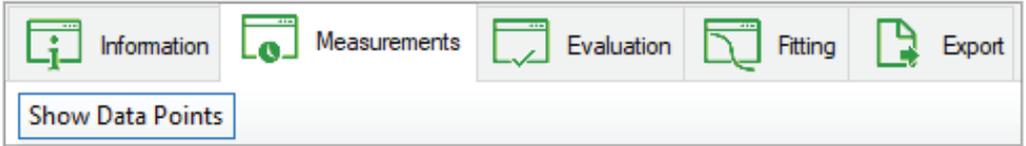


Figure 23 Data visualization options

In the toolbar above the graphs (Figure 23) the **Show Data Points** button is selectable on the **Measurement** tab. This button activates and deactivates the depiction of the individual measured data points as described in Section 4.3.3. This option is editable in both Public and Power User modes.

4.3.3 CONDUCTIVITY GRAPH

The upper graph shows the thermal conductivity (Figure 24). The graph shows the data points with one line. The x- and y-axes are automatically scaled to show all recorded data.

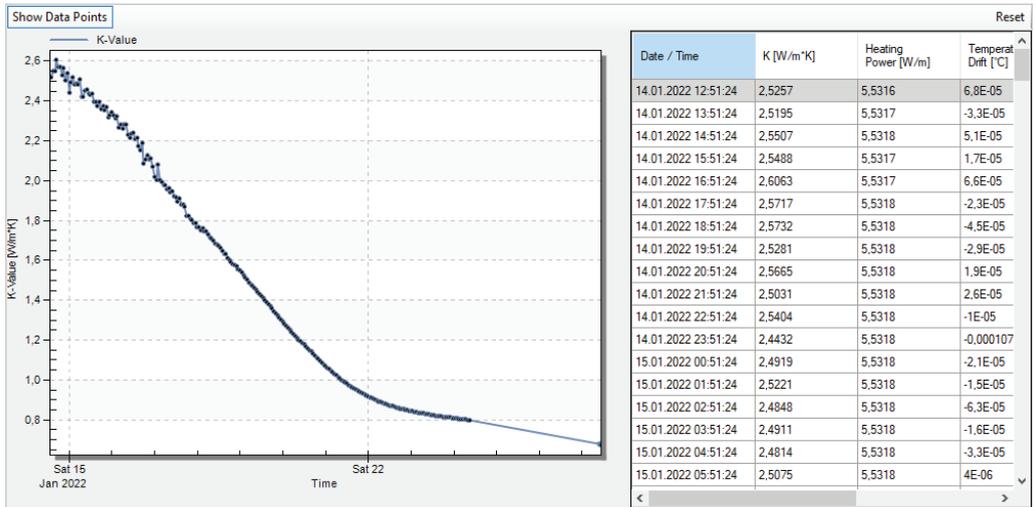


Figure 24 Upper graph

The temperature graph can be visualized by right-clicking the mouse and selecting the Show temperature graph option from the pop-up menu (Figure 25).

REGISTERS FOR PROCESSING DATA

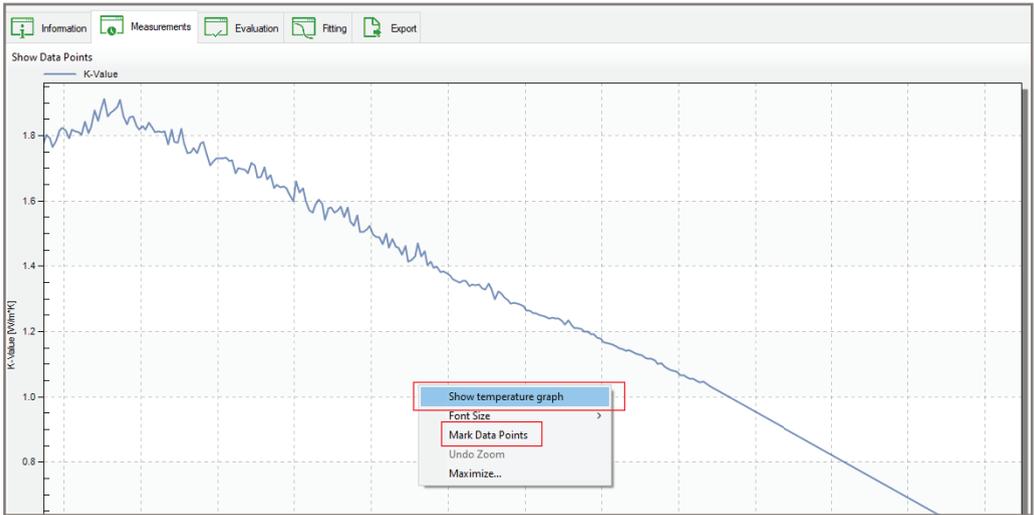


Figure 25 Pop-up dropdown menu

The temperature graph shows the changes of the thermal conductivity values as a line without individual dots for the data by default (Figure 26). If needed, a user can visualize all individually recorded data by moving the cursor on a line, right-clicking the mouse, and selecting **Mark Data Points** option from the context sensitive pop-up, dropdown menu (Figure 25). When this option is activated, single data points can be searched in the data table by clicking on a specific value in the graph. Data points can now be edited or deleted in the table (Power User only). When deselecting the option the individual data points disappear again. Another option for showing the data is clicking on the respective **ON-OFF** button in the toolbar line above the graph.

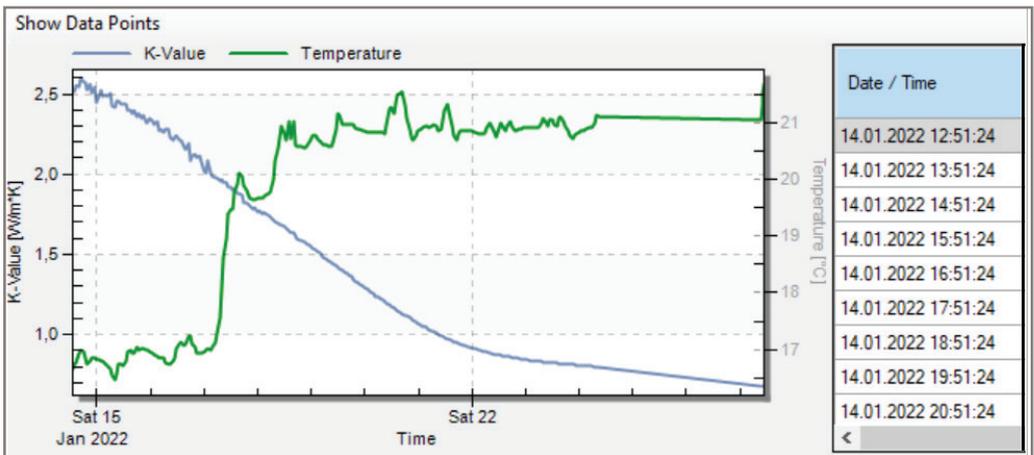


Figure 26 Temperature graph option

4.3.4 WEIGHT GRAPH (DRYOUT MEASUREMENT ONLY)

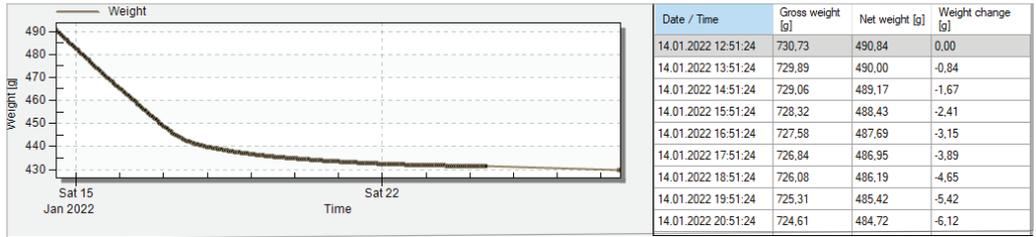


Figure 27 Lower graph—Weight graph

The lower graph (Figure 27) is the weight graph. It shows a gray 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 this data depends on the accuracy of the values for the setup parts (needle sensor, soil sampling ring, o-rings, sampling ring lid), and possible additional weights as described in the **Information** register tab. The relative accuracy of weight changes is dependent on the accuracy of the scale used.

The x- and y-axes are automatically scaled to show all recorded data. Parts of the graph can be manually enlarged and reset by right-clicking the mouse button and selecting the Maximize option in the pop-up menu.

NOTE: Changing the time axis of the weight graph does not affect the conductivity graph and vice versa. Visualization of the actual measured points can be activated and deactivated as described for the conductivity graph (Section 4.3.3).

Understanding the phases of evaporation are important for accurate interpretation of the weight data. In a typical measurement the weight data will first show a continuous weight loss at an almost constant rate that reflects the potential evaporation rate in the laboratory environment. Small changes in slope can be caused by temperature fluctuations in a lab and/or 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 (Figure 28). After Phase 1 evaporation, the rate drops and the slope of the weight curve becomes less steep. This is called Phase 2 Evaporation (Figure 28). The water loss rate is now controlled by the resistance of the drying soil near the soil surface.

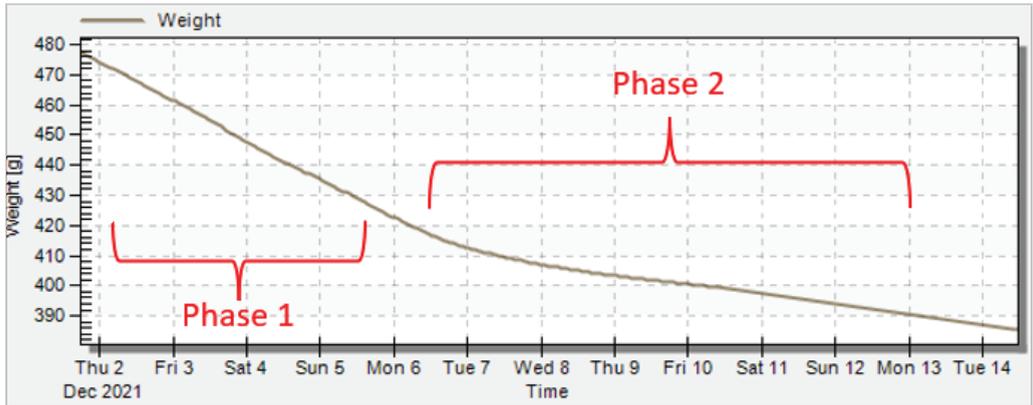


Figure 28 Phases of weight curve

4.3.5 CONDUCTIVITY DATA WINDOW

The window at the upper right (Figure 24) shows the recorded thermal conductivity data, together with the times, the heating power, the temperature drift, the start temperature, and the maximum temperature heat. The data can be edited by Power Users by hovering the cursor in the data window and right-clicking the mouse. Possible operations include deletion of lines, changes to contents, and displaying the heating curve of one consecutive conductivity measurement (Figure 29). Also, multiple lines can be selected and the data can be copied using the **Ctrl + c** keyboard combination. In Power User Mode deletion of data will immediately be shown in the graph on the left. By selecting one single measurement point in the graph, the table automatically switches to this measurement line.

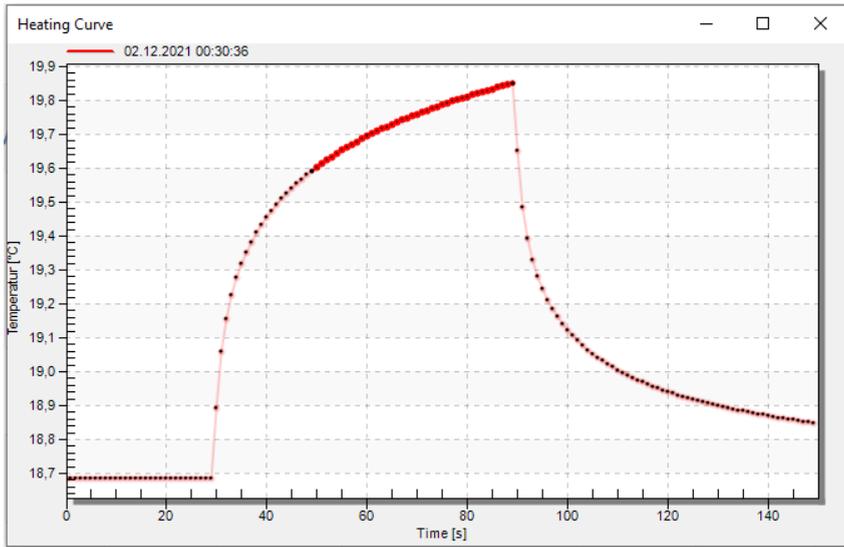


Figure 29 Heating curve

4.3.6 WEIGHT DATA WINDOW (DRYOUT MEASUREMENT ONLY)

The recorded weight data (Figure 27) is shown in the lower right of the weight data window. After date and time (column 1) the measuring system total weight, including all tare weights, is listed in column 2. The soil plus water net weight is calculated from the total weight minus the tare weights as specified in the **Information** register tab and displayed in column 3. These data are also depicted in the graph on the left side of the window. Finally, the net weight change from the start of the experiment is listed in column 4.

Scroll through the data window using the righthand scroll bar. By moving the cursor into the data window and right-clicking the mouse, the data can be directly edited by Power Users. Possible edits include deleting and changing individual data cell content. Also, multiple lines can be selected and the data can be copied (press the **Ctrl + c** keys). Manipulation of data or deletion of data (in Power User mode only) will immediately show in the graph on the left. If one measurement point in the graph is selected, the table automatically switches to the corresponding measurement line.

4.4 EVALUATION REGISTER (DRYOUT MEASUREMENT ONLY)

This section describes how the **Evaluation** register tab (Figure 30) is used when calculating thermal conductivity and water content data. The **Evaluation** register tab is used with dryout measurement only.

The **Evaluation** register shows three data groups in the upper part of the window that shows the specifications for the absolute water contents calculation, calculated parameters, and a menu where additional data points can be added. In the lower part of the window, a graph shows the resulting thermal conductivity data . The graph shows the VWC versus thermal conductivity (W/mK).

Right-click on the graph change the font size between small, medium, and large, and maximize the graph. Also, the water content display can be changed between volumetric or mass percent of water content.

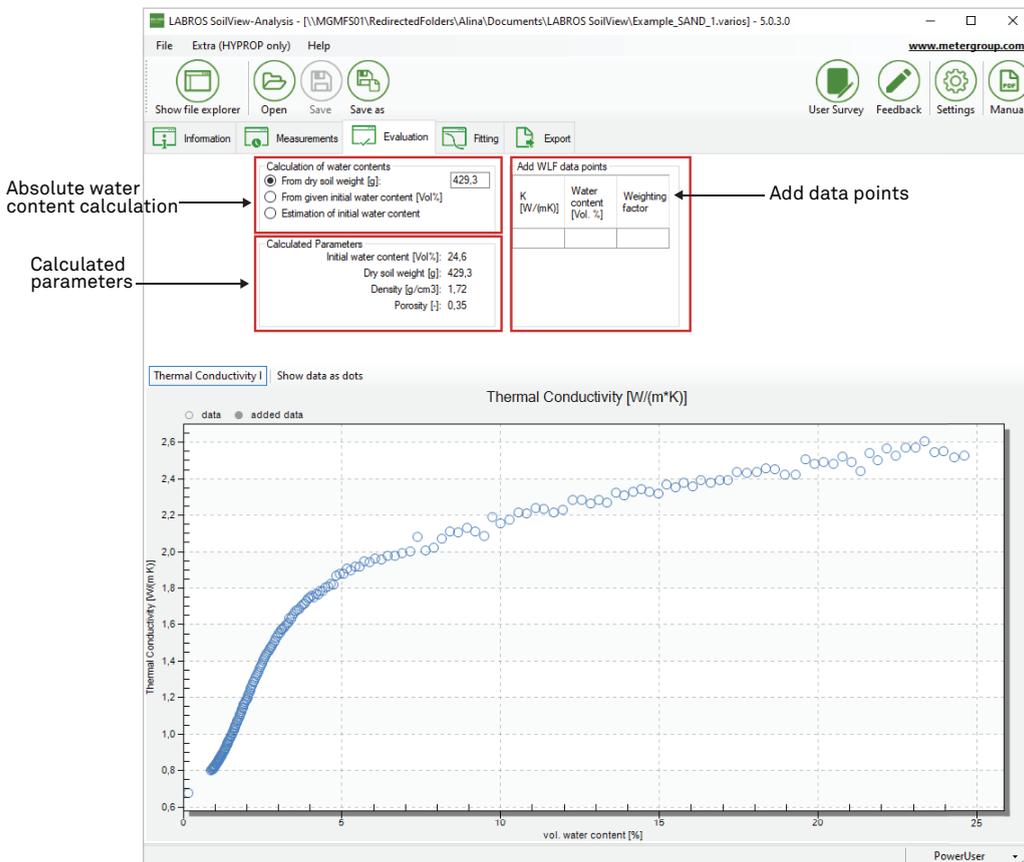


Figure 30 Evaluation register

4.4.1 ABSOLUTE WATER CONTENT EVALUATION

The relative shape of water content data is determined by the recorded weight change. The absolute level of water content data is affected by the parameters specified in the parameter group calculation of water contents.

OPTION 1: INITIAL WATER CONTENT CALCULATION FROM DRY SOIL WEIGHT

Calculation of water contents

From dry soil weight [g]: 429,3

From given initial water content [Vol%]

Estimation of initial water content

Figure 31 Water content calculation

The initial water content calculation from dry soil weight (Figure 31) is the best option if the dry soil weight has been determined after the end of the measurement by oven-drying at 105 °C for 24 h. The result accuracy depends on the precision of all involved parameters that are specified in the **Information** register. From the data additional physical parameters of the soil, such as the initial water content, the porosity, and the dry bulk density, are also calculated and shown in the **Calculated Parameters** group.

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 32 User-set water content calculation

The user-set initial water content external setting (Figure 32) allows a user to externally set the initial water content to a specific value from wherever this value is determined.

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 33 Initial water content estimation

If the soil dry weight is not available, option 3 can be used to automatically estimate the initial water content measurement (Figure 33). The LABROS SoilView-analysis software estimates water content assuming full saturation of the pore space (i.e., initial saturation = 100%). In practice this will rarely be reached; therefore, the calculated water content must be seen as an approximation of the true water content. As a result of this assumption, the initial water content, porosity, bulk density, and the dry soil weight can be calculated. These values are shown in the **Calculated Parameters** group.

If the mode of the initial water content is changed, the user-edited values for the dry soil weight and for initial water content remain in storage. This allows the user to switch between the options and to 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. **For these reasons Option 3 is not usually recommended.**

IMPORTANT: The calculation of porosity and absolute water content depends on all specified parameters in the Information register being correct. Any error in the data of the dry bulk density (default = 2.65 g/cm³), the mass of the sampling ring containing the sample, and mass of dry soil specified in the Evaluation register will be linearly transferred to the results.

IMPORTANT: Overfilling or underfilling the sampling rings with soil will cause appreciable errors. As a general guideline, a 1-mm error in sample weight causes an approximate 2% error in the calculated data.

4.4.2 ADDING INDEPENDENT CONDUCTIVITY DATA

Add WLF data points		
K [W/(mK)]	Water content [Vol. %]	Weighting factor

Figure 34 Add independent conductivity data

Users can add independently measured data from the METER TEMPOS and other devices measuring thermal conductivity (Figure 34).

Right-click the blank editing field and select one of the option in the pop-up menu that appears (Figure 35):

Insert row
Delete row
Delete content

Figure 35 Pop-up menu

The data points entered from independently measured data are displayed as filled dots in the graph, and data measured by the VARIOS are shown as empty circles.

Carefully select the appropriate units when adding data:

- thermal conductivity must be added in W/mK units
- VWC only be added as a percentage.

NOTE: Make sure to use the correct regional conventions for the decimal separator (comma or period). Added data can be edited and deleted.

4.5 FITTING REGISTER (DRYOUT MEASUREMENT ONLY)

This section describes how the **Fitting** register tab fits thermal conductivity functions to the data. The **Fitting** register tab is used with dryout measurement only. Model selection and function parameters are available in the **Fitting** register tab (Figure 36).

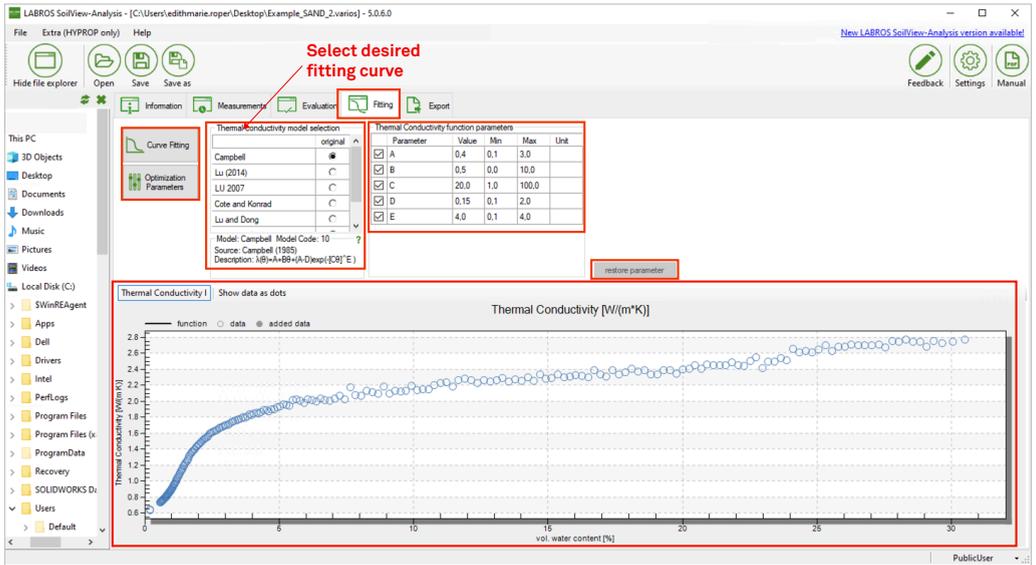


Figure 36 Fitting register

For use in numerical modeling, thermal characteristics are described by parametric functions for $\lambda(\theta)$ and $C(\theta)$, where θ (m^3/m^3) is the VWC, λ ($\text{W m}^{-1} \text{K}^{-1}$) the thermal conductivity, and C ($\text{J m}^{-3} \text{K}^{-1}$) the thermal capacity. LABROS SoilView-Analysis software provides a high-class algorithm to fit a variety of functional relationships of the $\lambda(\theta)$ curve to the data (C is the sum of the head capacities of the mineral, the organic, and the liquid phases). No specification of initial guesses for the parameter values is required. Six widely-used conductivity models are available. All models are described in [Appendix A](#).

4.5.1 FITTING FUNCTIONS

The **Fitting** register tab has the **Curve Fitting** button (Figure 36), as well as the **Optimization Parameters** button on the left (allows user to edit the optimization parameters), and the **Restore Parameters** button on the right. The data to be fitted is shown together with the fitting function in the graph in the lower part of the window. The **Restore Parameters** button will reset all values for the parameter bounds to the default values.

To fit the selected function to the data left-click on the **Curve Fitting** button. A window will pop up (Figure 37) that indicates that the fitting routine is running. This process will last only a few seconds and cannot be stopped or otherwise interrupted.

NOTE: In some cases the fitting process will work continuously and not lead to completion. In these cases the user can cancel the process in the Windows Task Manager.

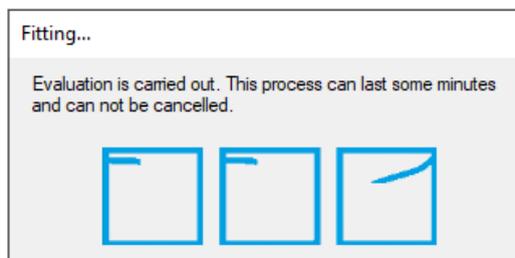


Figure 37 Fitting process window

The fitting algorithm minimizes the sum of squares deviations between data points and fitted functions using a global optimization scheme.

4.5.2 SELECTING A FITTING MODEL AND PARAMETER BOUNDS

A fitting model is selected by left-clicking in the radio button next to the desired fitting model on the **Fitting** register window. By default all model parameters are included in the fitting process (except parameter **ths** for model LU 2007 and Cote and Konrad; Appendix A) and are 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. For most soils this will not be necessary. In some cases users may have prior knowledge about parameters that can lead to greatly reduced bandwidths and changing the parameters based on prior knowledge will speed up the convergence of the algorithm.

To change the default minimum and maximum parameter values type the new value into the respective field in the group **Thermal Conductivity function parameters**. To store a typed value the cursor must be moved out of the field either by pressing the **Tab** or **Return** key or by moving the mouse to another field. Default values can be restored by selecting the **Restore Parameters** button.

If the checkbox in front of the parameter is selected, the value will be automatically calculated. By unchecking the checkbox the default value shown can be overwritten with a new value entered manually. If a model selection is changed, the user will be prompted to confirm whether they want to continue with the new value for the fitting parameter or not.

4.5.3 FITTING PARAMETER ESTIMATION AND UNCERTAINTY MEASURES

After the fitting process is complete, the parameter fields switch from the **Input** mode to the **Results** mode (Figure 38). In **Results** mode the optimized parameters are shown in the previously empty column with the Value fields and the uncertainties of the individual parameters 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 provided in Appendix C. For fixed parameters the uncertainty is zero.

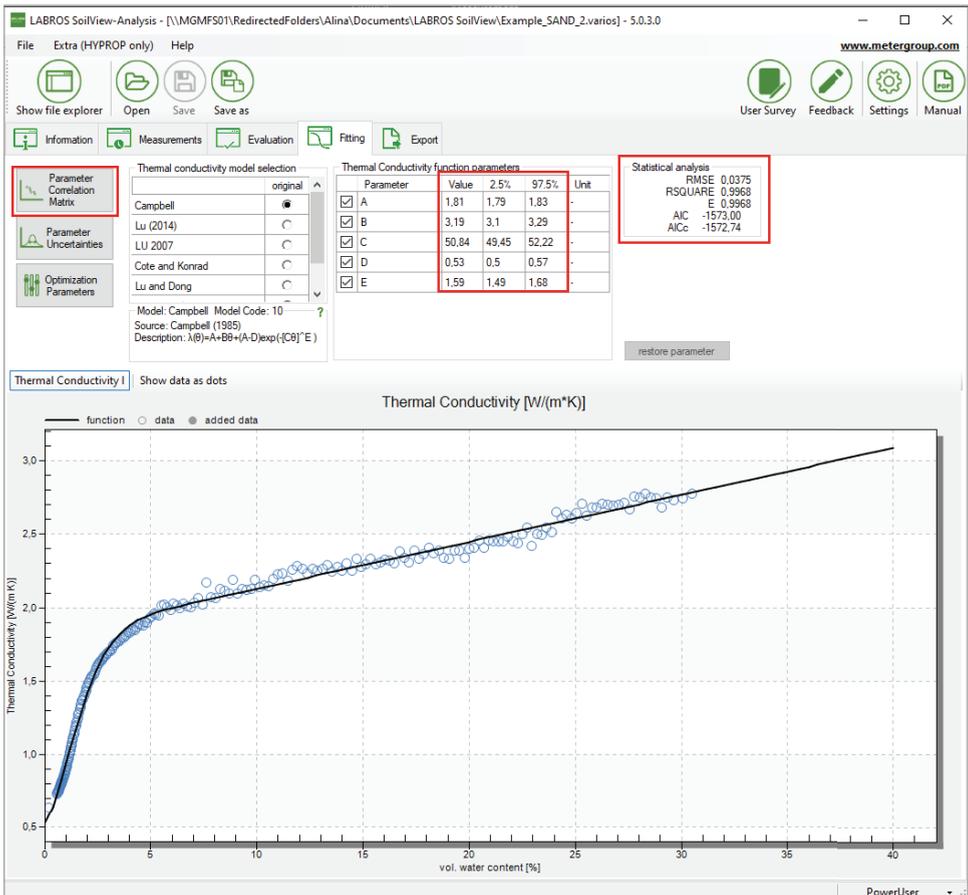


Figure 38 Fitting register Results mode

The quality of the fit is quantified in the group **Statistical analysis** in the upper right and can be visually inspected from the graph. Fit quality is given in terms of the root mean square error (RMSE). The RMSE is an indication of the mean distance between a data point and the fitted function. An RMSE of 0.01 for the thermal conductivity data fit indicates an average distance of the fitted curve to observed data of $W\ m^{-1}\ K^{-1}$. Additionally, the coefficient of determination (r^2) and the Nash-Sutcliffe Index (E) are displayed. Models with a higher number of parameters are generally more flexible, and 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 software shows the corrected Akaike Information Criterion (AICc, Akaike, 1974; Hurvich, Tsai, 1989) in the **Statistical analysis** group. This criterion accounts for the different number of adjustable parameters when selecting the best model. The value will normally be negative. The more appropriate model is one with the smallest value (i.e., the larger the absolute number).

NOTE: The actual value of the AICc has no meaning. It can only be used to compare different fitting models for one set of data. For details on the statistical criteria see [Appendix C](#).

As indicated above, models with a higher number of parameters are generally more flexible but they will have a higher correlation between the optimized parameters and higher uncertainties for the individual parameters. Pressing the **Parameter Correlation Matrix** button will cause the parameter **Correlation Matrix** window to appear ([Figure 39](#)).

Correlation Matrix				
	ldry	lsat	thf	m
ldry	1.000	0.000	0.000	0.000
lsat	1.000	1.000	0.000	0.000
thf	0.764	0.783	1.000	0.000
m	-0.979	-0.984	-0.878	1.000

Figure 39 Correlation matrix window

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 another parameter; 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 indicate a quality fitting problem. A parameter correlation that is too high indicates an overparameterization of the selected model and is undesirable.

4.5.4 FUNCTION GRAPHS

In the lower part of the **Fitting** register window a graph appears containing the calculated VARIOS data, the entered data, and the fitted conductivity function. As with any other graphs in the LABROS SoilView-Analysis software, the graph can be magnified to full screen or zoomed in by selecting the respective option in the context-sensitive submenu. Right-click the mouse to access zoom or full screen viewing for the graphs.

The fitted functions will disappear from the screen if either parameter settings are changed (e.g., by modifying the permissible data range), or if a setting in another register is changed that affects the calculated VARIOS data. After the fitting process, the fitting results can be exported as explained in the **Export** register ([Section 4.6](#)).

4.5.5 MODIFYING OPTIMIZATION PARAMETERS

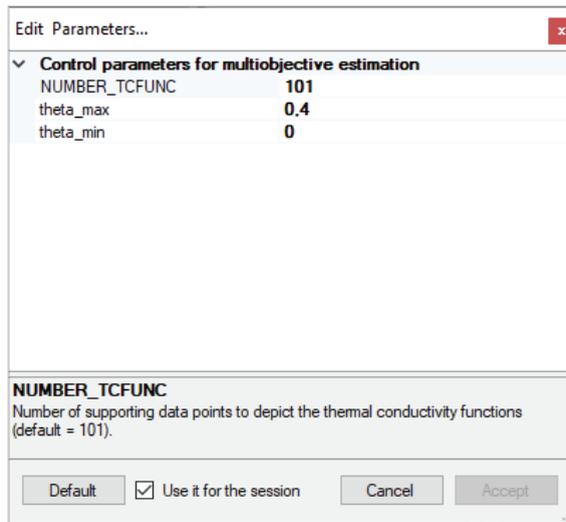


Figure 40 Edit Fitting parameters

Users can edit some of the parameters ([Figure 40](#)) that specify the calculations and the depiction of the fitted function. The specifications are listed by selecting the **Optimization Parameters** button and are described in [Table 10](#).

Table 10 Fitting parameters options

Variable	Explanation	Data Value	Editable	
			Public User	Power User
NUMBER_TCFUNC	Number of points for the displayed and exported conductivity function.	101	Yes	Yes
theta_max	Upper limit of water content range to calculate thermal conductivity functions (default: maximum measured water content).	0.6	Yes	Yes
theta_min	Lower limit of water content range to calculate thermal conductivity functions (default 0)	0	Yes	Yes

4.6 EXPORT REGISTERS

The **Export** register tab (Figure 41) enables all graphs, raw data, calculated data, fitted functions, and other parameters of interest to be exported. User specifications for data format, file name convention, and directory will be kept as default as long as the user remains in the session.

LABROS SoilView-Analysis supports the Microsoft Excel® output file format (*.xlsx). The Excel file will contain all relevant data in different worksheets:

- Configuration and information
- Measured data
- Evaluation of measured conductivity data (dryout measurement only)
- Fitted conductivity data (dryout measurement only)
- Parameters of fitted models (dryout measurement only)
- Correlation matrix of fitted data (dryout measurement only)
- Statistical analysis (dryout measurement only)
- Measured raw data (if specified)

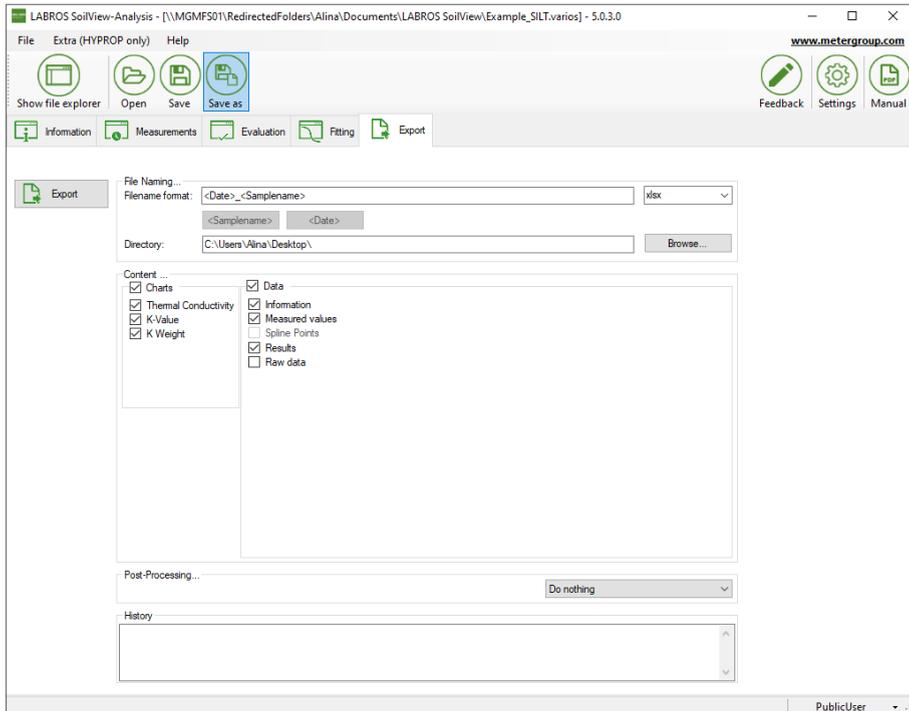


Figure 41 Export register

4.6.1 OUTPUT SETTINGS

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

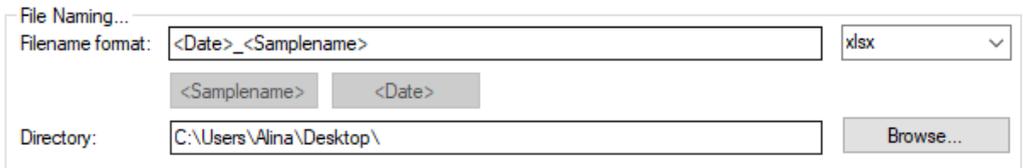


Figure 42 Export data filename

Enter the output filename in the **Filename format** field (Figure 42). All permitted characters can be used in the filename. The two default settings **<Date>** and **<Sample name>** are available for optional use in any position within the filename. They will automatically be replaced by the current date or sample name.

Directory:	<input type="text" value="C:\Users\Alina\Desktop\"/>	<input type="button" value="Browse..."/>
------------	--	--

Figure 43 Directory

Enter the output directory in the **Directory** field (Figure 43) or click on the **Browse** button to select a directory.

4.6.2 CONTENT

In the **Content** window (Figure 44) select the checkboxes for the charts and the data that should be exported.

NOTE: Exporting raw data is deselected by default. When exporting the raw data, select the Raw data checkbox.

Content ...	
<input checked="" type="checkbox"/> Charts <input checked="" type="checkbox"/> Thermal Conductivity <input checked="" type="checkbox"/> K-Value <input checked="" type="checkbox"/> K Weight	<input checked="" type="checkbox"/> Data <input checked="" type="checkbox"/> Information <input checked="" type="checkbox"/> Measured values <input type="checkbox"/> Spline Points <input checked="" type="checkbox"/> Results <input type="checkbox"/> Raw data

Figure 44 Content window checkboxes

4.6.3 POSTPROCESSING

In the **Postprocessing** group set different actions that should be executed either after exporting or while exporting (Figure 45).

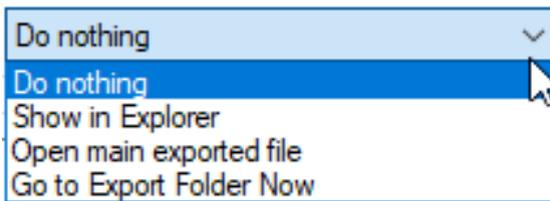


Figure 45 Postprocessing

4.6.4 HISTORY

The **History** group (Figure 46) provides an overview of all recently executed exports.

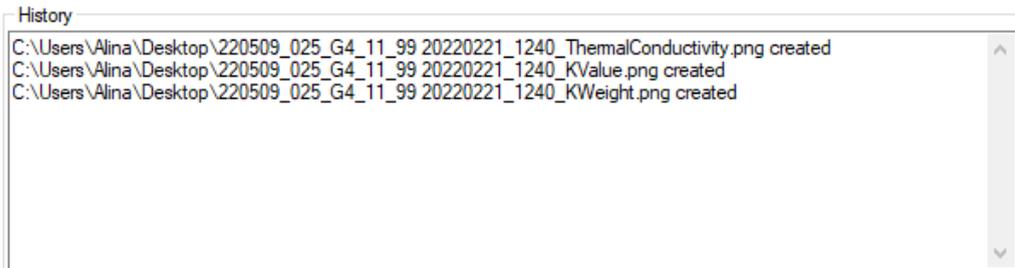


Figure 46 History group

5. SERVICE

5.1 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

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sales.europe@metergroup.com

Phone: +49 89 12 66 52 0

Fax: +49 89 12 66 52 20

Website: metergroup.com

If contacting METER by email please include the following information:

Name	Email address
Address	Instrument serial number
Phone	Description of the problem

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5.2 TERMS AND CONDITIONS

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APPENDIX A. THERMAL CONDUCTIVITY THEORY

This appendix contains an overview of thermal conductivity theory, functions, and thermal conductivity courses.

Thermal conductivity of porous media, such as soils, depends on mineralogy, organic matter content, bulk density, and water content. The water content is highly variable within short time intervals (days to months), whereas the other variables can be regarded as constant. Therefore, typical models for thermal conductivity describe the relationship between thermal conductivity λ ($\text{W m}^{-1} \text{K}^{-1}$) and VWC θ (m^3/m^3).

There are two ways to derive the values of the model parameters:

- Predicting values by means of known soil properties (on mineralogy, organic matter content, bulk density).
- Using measured data for $\lambda(\theta)$ and estimating the parameters by nonlinear regression.

The LABROS SoilView-Analysis software applies the latter approach.

In order to empirically describe the $\lambda(\theta)$ relation, Johansen (1975) introduced a normalized thermal conductivity function, called Kersten number: $K_e = (\lambda(\theta) - \lambda_{dry}) / (\lambda_{sat} - \lambda_{dry})$, where λ_{dry} and λ_{sat} are thermal conductivities at oven dryness or saturation, respectively. The dimensionless $K_e(\lambda)$ relation was described by a simple logarithmic function. This model type was adopted by several authors with different descriptions of $K_e(\lambda)$ (Cote and Konrad, 2005; Lu et al., 2007; Lu and Dong, 2015). The general form of this function type is:

$$\lambda(\theta) = \lambda_{dry} + K_e (\lambda_{sat} - \lambda_{dry}) \quad \text{Equation 1}$$

Figure A.1 shows the course of these kinds of functions for the Lu et al., (2007) (left) and Cote and Konrad (2005) (right) formulations (details of the models are given in Appendix B).

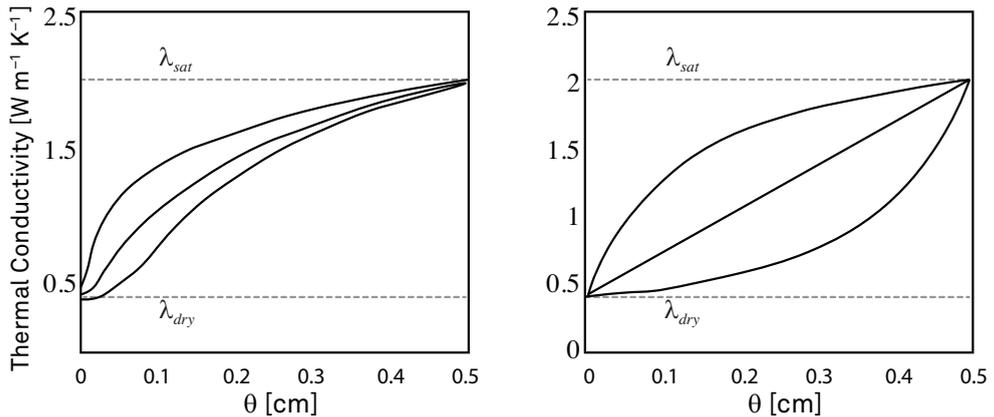


Figure A.1 Thermal conductivity courses for Lu et al., and Cote and Konrad

Figure A.1 shows typical courses of the Lu et al. (2007) (left) and Cote and Konrad (2005) (right) thermal conductivity models using the Johansen (1975) approach. The parameter varied for the Lu et al. (2007) model was α (0.5 0.9 1.1). The parameter varied for the Cote and Konrad (2005) model was κ (0.2 1.0 5.0).

Besides these Johansen type functions there are some other models, such as the predictive model of Campbell (1985) and the empirical model of Chung and Horton (1987), which are both implemented in the HYDRUS-1D and HYDRUS 2/3-D software packages (Simunek et al. (2013) and Simunek et al. (2006)). All models implemented in the LABROS SoilView-Analysis software are listed in Appendix B. The model of Campbell (1985) is particularly well suited to describe thermal conductivity functions for sands because of its flexibility and general shape.

Figure A.2 shows the courses of the Campbell model for typical soils (details of the models are given in Appendix B).

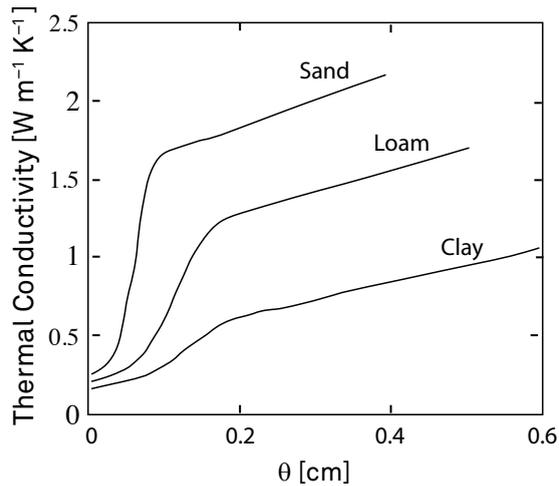


Figure A.2 Thermal conductivity courses for Campbell

Figure A.2: Typical courses of the Campbell (1985) thermal conductivity model for three different textures. Parameters for A, B, C, D, and E are: 1.5, 1.7, 15.0, 0.25, and 4.0 for the sand, 1.0, 1.4, 8.0, 0.2, and 4.0 for the loam and 0.4, 1.1, 7.0, 0.15, and 4.0 for the clay, respectively.

APPENDIX B. FREQUENTLY USED MODEL TYPES

This section provides and explains nine different model types that are frequently used.

Johansen (1975)

$$\lambda(\theta) = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry})[A \ln(S) + B]$$

Equation 2

with $\lambda_{dry}(W m^{-1} K^{-1})$, $\lambda_{sat}(W m^{-1} K^{-1})$, $A(-)$ and $B(-)$ as fitting parameters and $S(-)$ is saturation defined as θ divided by θ_s where $\theta_s(-)$ is the saturated water content. In order to guarantee that $\lambda = \lambda_{sat}$ at saturation, B should be set to unity. Since $\ln(S)$ becomes very negative at low values for S , the Johansen model is meaningless close to oven dryness. The model is currently implemented in a way that if $\lambda < \lambda_{dry}$, λ becomes λ_{dry} .

Lu et al. (2007)

$$\lambda(\theta) = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry}) \exp(\alpha[1 - S^{\alpha-1.33}])$$

Equation 3

with $\lambda_{dry}(W m^{-1} K^{-1})$, $\lambda_{sat}(W m^{-1} K^{-1})$, and $\alpha(-)$ as fitting parameters and $S(-)$ is saturation defined as θ divided by θ_s where $\theta_s(-)$ is the saturated water content.

Cote and Konran (2005)

$$\lambda(\theta) = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry}) \frac{\kappa S}{1 + (\kappa - 1)S}$$

Equation 4

with $\lambda_{dry}(W m^{-1} K^{-1})$, $\lambda_{sat}(W m^{-1} K^{-1})$, and $\kappa(-)$ as fitting parameters and $S(-)$ is saturation defined as θ divided by θ_s where $\theta_s(-)$ is the saturated water content.

Lu and Dong (2015)

$$\lambda(\theta) = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry}) \left\{ 1 - \left[1 + \left(\frac{\theta}{\theta_f} \right)^m \right]^{\frac{1}{m}-1} \right\}$$

Equation 5

with $\lambda_{dry}(W m^{-1} K^{-1})$, $\lambda_{sat}(W m^{-1} K^{-1})$, $m(-)$, and $\theta_f(-)$ as fitting parameters.

He et al. (2017)

$$\lambda(\theta) = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry}) [A e^{\theta-B}]^{-1}$$

Equation 6

with $\lambda_{dry}(W m^{-1} K^{-1})$, $\lambda_{sat}(W m^{-1} K^{-1})$, $A(-)$, and $B(-)$ as fitting parameters.

Campbell (1985)

$$\lambda(\theta) = A + B\theta - (A - D)\exp(-[C\theta]^E) \quad \text{Equation 7}$$

with $A(W m^{-1} K^{-1})$, $B(W m^{-1} K^{-1})$, $C(-)$, $D(W m^{-1} K^{-1})$, and $E(-)$ as fitting parameters. These parameters can also be derived from soil properties and mineralogy. As can be easily seen, $D = \lambda_{dry}$ thermal conductivity at $\theta=0$. The model of Campbell is very flexible and can be used to describe almost every data set as long as the $\lambda(\theta)$ is monotonously increasing. Parameter E is usually fixed at 4.0.

Lu et al. (2014)

$$\lambda(\theta) = \lambda_{dry} + \exp(\beta - \theta^\delta) \quad \text{Equation 8}$$

with $\lambda_{dry}(W m^{-1} K^{-1})$, b and d as fitting parameters.

Chung and Horton (1987)

$$\lambda(\theta) = \lambda_{dry} + b_2\theta + b_3\theta^2 \quad \text{Equation 9}$$

with $\lambda_{dry}(W m^{-1} K^{-1})$, $b_2(W m^{-1} K^{-1})$, and $b_3(W m^{-1} K^{-1})$ as fitting parameters.

APPENDIX C. PARAMETER ESTIMATION

The following explains and defines the objective function for parameter estimation.

The parametric models for $\lambda(\theta)$ are fitted to the data points. The fitting is accomplished by a nonlinear regression algorithm by minimizing the sum of weighted squared residuals between model prediction and data pairs:

$$\Phi(b) = \sum_{i=1}^r W_{\lambda,i} \left[\bar{\lambda}_i - \hat{\lambda}_i(b) \right]^2$$

Equation 10

where r is the number of data pairs of $\lambda(\theta)$, $W_{\lambda,i}$ are the weights of the individual data points, in case of fitting only one data type often set to unity, and $\bar{\lambda}_i$ and $\hat{\lambda}_i(b)$ are the measured and model predicted values, respectively, and b is the parameter vector.

The parameter estimation procedure must guarantee that the best parameter combination for the appropriate model 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 depend on the initial guesses. Therefore, the software uses the shuffled complex evolution algorithm (SCE) (Duan et al., 1992), which is a global parameter estimation algorithm.

APPENDIX D. POSTPROCESSING DIAGNOSTIC VARIABLES

The first measure to evaluate the performance of the fitted model is the objective function values at their estimated minimum, Φ_{min} . This is 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:

$$RMSE = \sqrt{\frac{1}{r} \sum_{i=1}^r [Y_i - \widehat{Y}_i]^2}$$

Equation 11

where y_i and \hat{y}_i are measured and model predicted quantities, i.e., thermal conductivities. 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 also calculated. The Nash-Sutcliffe index is given by Equation 12:

$$E = 1 - \frac{\sum_1^r [y_i - \widehat{y}_i]^2}{\sum_1^r [y_i - \bar{y}_i]^2}$$

Equation 12

where \bar{y}_i is the mean measured quantity. In Equation 13 the coefficient of determination (r^2) is given by:

$$r^2 = 1 - \frac{\sum_1^r [y_i - \bar{y}_i][\widehat{y}_i - \bar{\widehat{y}}_i]}{\sqrt{\sum_1^r [y_i - \bar{y}_i]^2 [\widehat{y}_i - \bar{\widehat{y}}_i]^2}}$$

Equation 13

To account for the different number of adjustable parameters when comparing different models fitted to the same data, LABROS SoilView-Analysis software 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 as described by Ye et al. (2008):

$$AIC = n \ln(\Phi_{min}/n) + 2k$$

Equation 14

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:

$$AICc = n \ln(\Phi_{min}/n) + 2k + \frac{2k(k+1)}{n-k-1} \quad \text{Equation 15}$$

where $n \ln(\Phi_{min}/n)$ penalizes a poor fit, $2k$ is the number of parameters, and $2k(k+1)/(n-k-1)$ is the correction for small values of n/k . If n/k becomes large the [super fraction] becomes negligible and the $AICc$ converges to AIC .

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

$$BIC = n \ln(\Phi_{min}/n) + k \ln(n) \quad \text{Equation 16}$$

and

$$KIC = (n - k) \ln(\Phi_{min}/n) - k \ln(2\pi) + \ln |J^T W| \quad \text{Equation 17}$$

Where $|J^T W|$ is the determinant of the Fisher information matrix. J is the Jacobian or sensitivity matrix with elements $J_{i,j} = \partial \widehat{Z}_i / \partial b_j$ where \widehat{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 w is the weighting matrix.

APPENDIX E. UNCERTAINTY ANALYSIS

E.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 (Omlin and Reichert, 1999):

$$C_p \approx \frac{\Phi_{\min}}{n-k} (J^T W J)^{-1} \quad \text{Equation 18}$$

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

$$\hat{b}_i \pm \sqrt{C_{pi,i} \times t_{n-k,\alpha/2}} \quad \text{Equation 19}$$

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

E.2 FUNCTION UNCERTAINTIES

The uncertainties for the $\lambda(\theta)$ functions are determined by calculating the covariance of the model response, C_z :

$$C_z \approx J^T C_p J \quad \text{Equation 20}$$

where the J is the Jacobian or sensitivity matrix with elements $J_{i,j} = \partial \hat{Z}_i / \partial b_j$, where \hat{Z}_i is the model prediction at point i and b_j is the j th parameter. The confidence interval for the model output is given by:

$$\hat{y}_i \pm \sqrt{C_{zi,i} \times t_{n-k,\alpha/2}} \quad \text{Equation 21}$$

where \hat{y}_i is the model output $\hat{\lambda}_i$. Again, α is set to 0.05 leading to the 95% confidence intervals for the functional relationships.

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