Manual

MultiSens-Software

Version 4.0

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Introduction

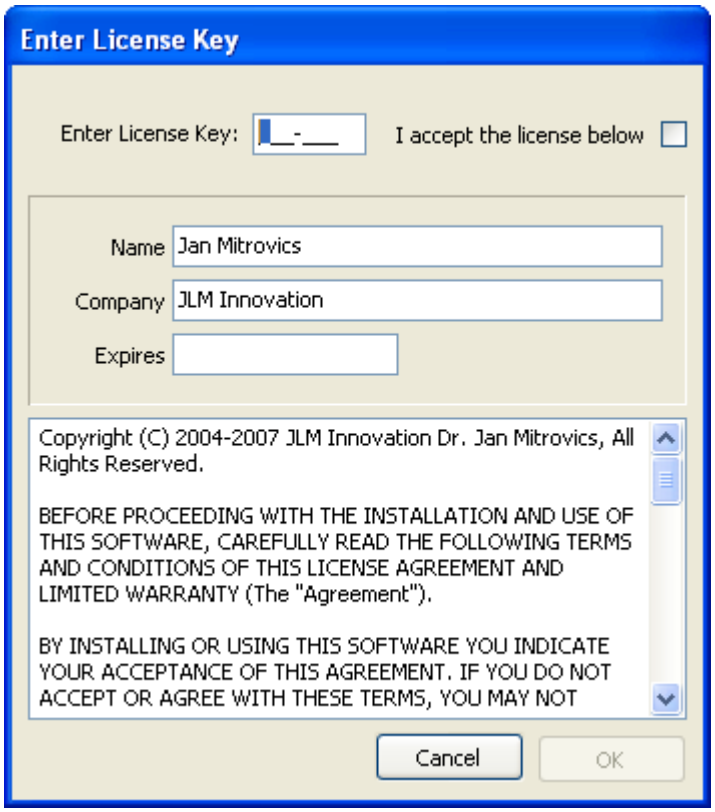
General

This operating manual describes the MultiSens software package. It addresses customers who are already familiar with the basics of chemical sensing combined with the numerical recognition algorithms.

Text positions which are characterized in this way should always be read through carefully before initiation of a system. In the case of nonobservance of these references, JLM Innovation GmbH and/or its reseller undertake no liability.

Installation

Typically this program is delivered as an executable setup file (setup.exe). Starting setup.exe will guide you through a simple set of dialogs to install MultiSens on your PC.

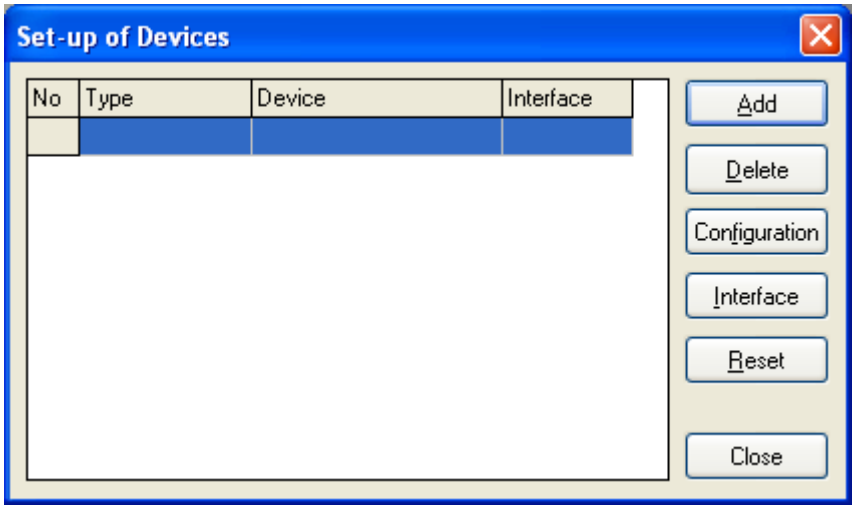


If the installation was carried out successfully, you can continue directly to work with your system. A re-start of Windows is not required.

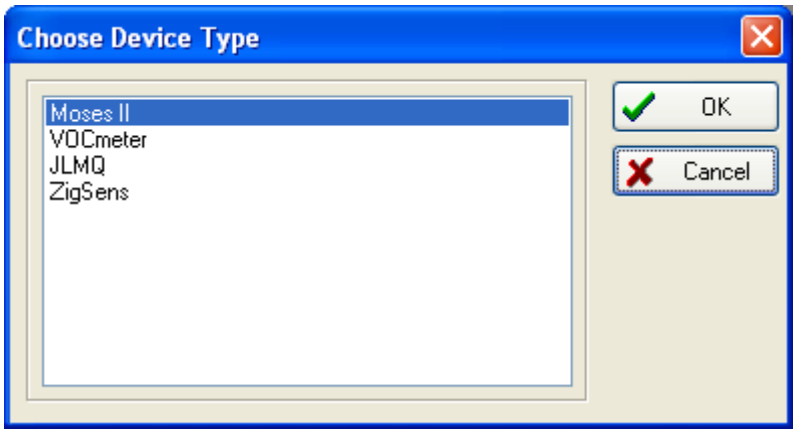
When you are first running MultiSens, you will be prompted with a license dialog. In order to proceed, you have to enter the License Key and click checkbox next to “I accept the license below”.

Configuration of the devices

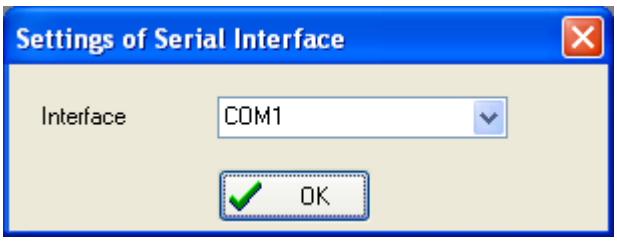
Before using any devices to perform measurements for the first time, you will have to tell MultiSens, which devices are attached to your computer. Start the program MultiSens and then choose the menu item **Options – Set-up of Devices**. A dialog box opens up in which you can add devices to a list.



Several devices may be added to this list. MultiSens will control all these devices simultaneously. This allows to create complex measurement set-ups with several different device measuring on the same sample. To add a device click on the **Add** button. A dialog will open, that allows you to select the type of device (the types of device may vary with the version of MultiSens installed on your computer):



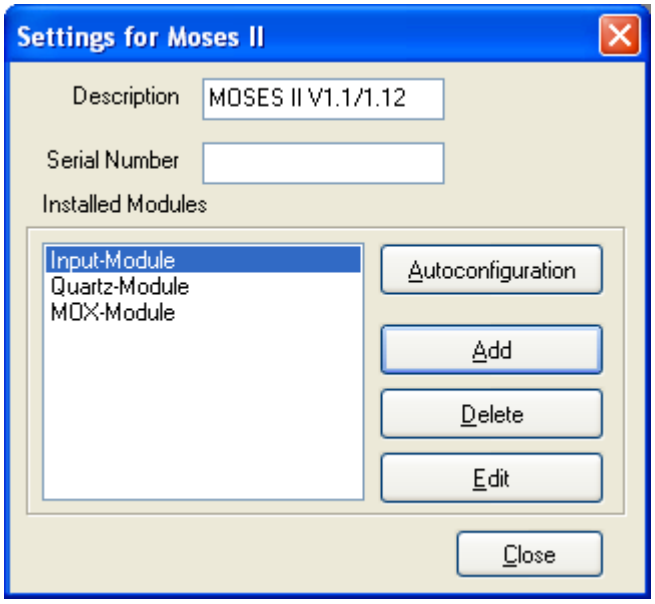
Select the appropriate device and press **Ok**. Depending on the device type you may be prompted with further dialogs, e.g. to identify a Com port that the device is connected to.



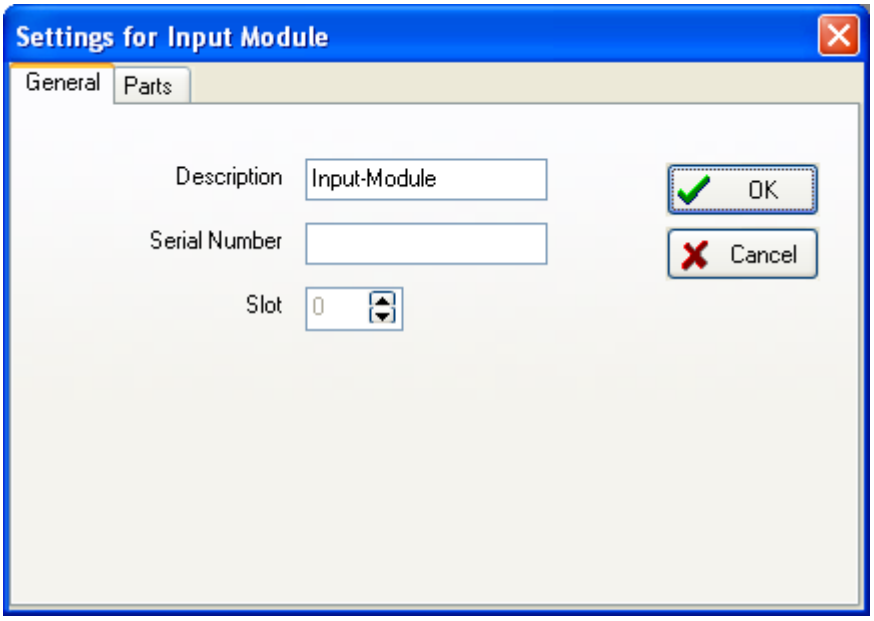
Some devices may have different configurations. E.g. a MOSES II instrument may have various modules installed. If supported by the device, MultiSens will retrieve all configuration information and default parameters directly from the attached device.

Some devices require manual configuration settings. Press the **Configuration** Button in the **Set-up of Device** dialog to view or change configuration settings.

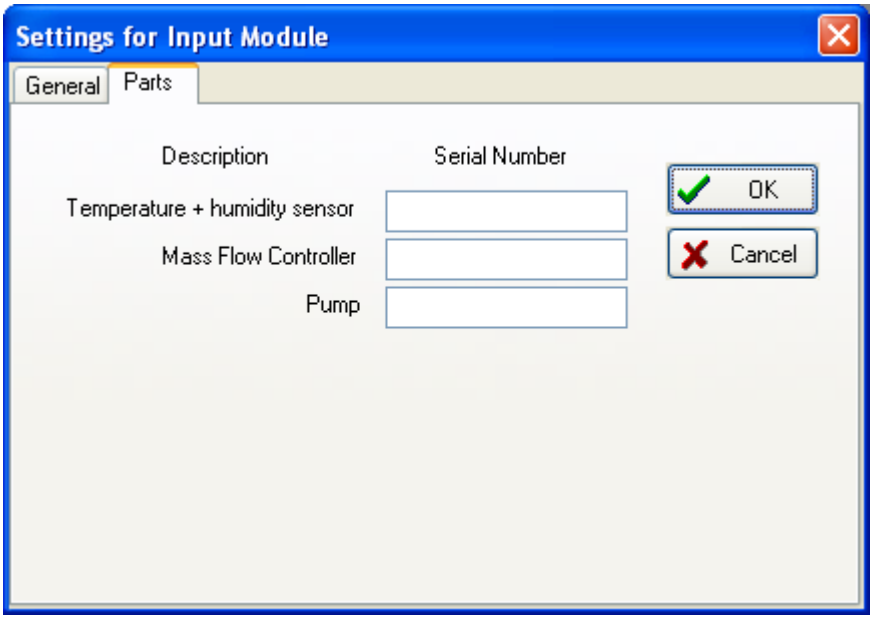
If you connect a MOSES II system, a window appears showing the following basic configuration:



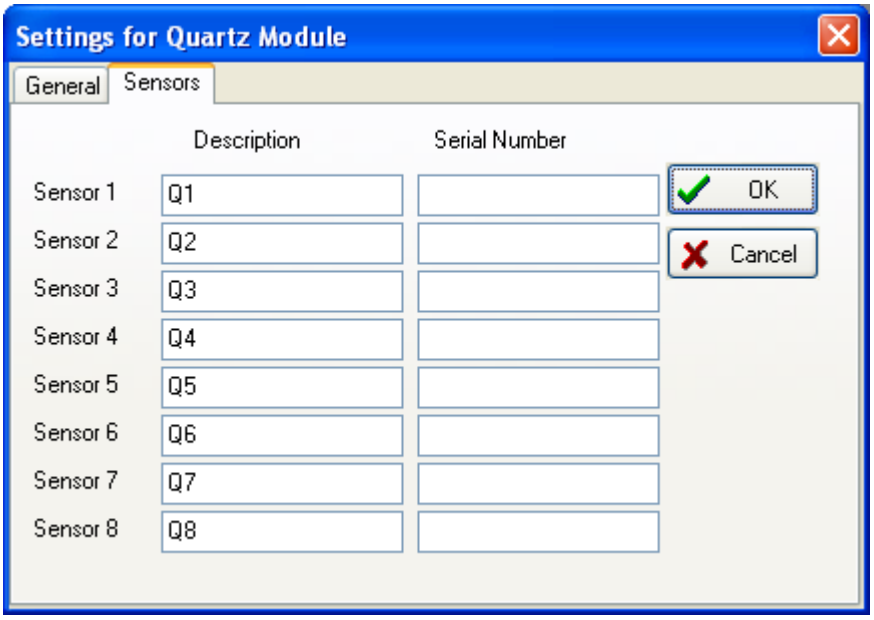
If you press Autoconfiguration the software will try to connect to the MOSES II – device and download the configuration information. Unlike the VOCmeter systems a MOSES II is a modular system where hardware modules with sensors or other functions can be installed by the user. The installed modules will be identified by the Autoconfiguration routine. The individual settings however can be edited and changed by the user. A page for general settings exists for all MOSES II modules. In the next screenshot this page is shown.



The text entered in description is predefined, but may be changed by the user. It will appear in all places of the software where a selection between different modules can be made. If two modules of the same type are installed in a MOSES II system it is advised to changes this description (e.g. by adding a number) to be able to more easily discriminate the modules.



In case of the input module on the module specific page only serial numbers might be introduced for the components of the input module.

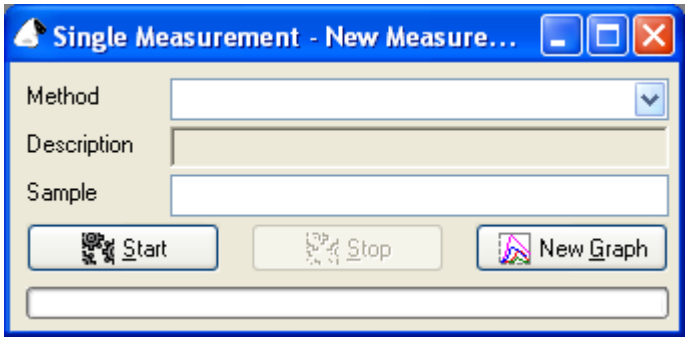


In the case of a sensor module (e.g. the quartz module) for each sensor description and serial number can be entered. The description of the sensor will be used in all places the software identifies a sensor (e.g. as Label on a graph, in sensor selection dialogs, etc.). By default the sensors in a module are identified by a letter (identifying its type) and a number (identifying its position). If two modules of the same type are present this will lead to possible confusion as two sensors will have the same description. In this case it is advised to change the sensor descriptions of one module.

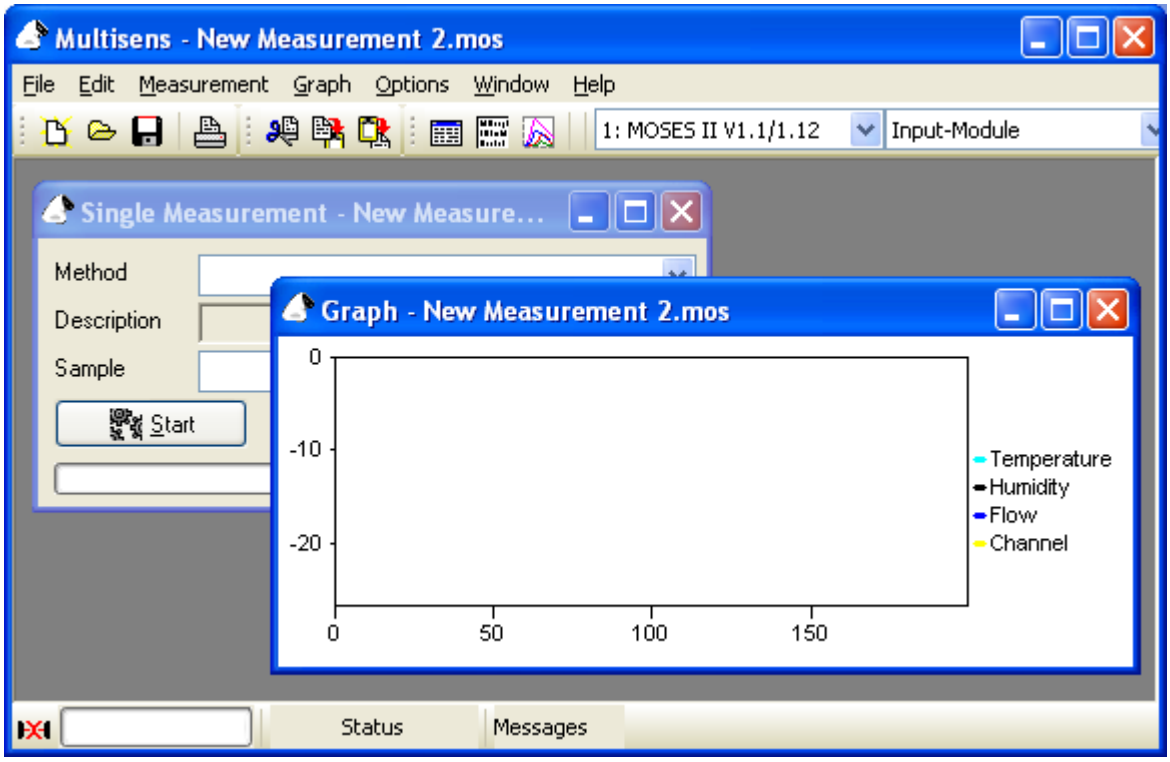
MultiSens step by step

Run a single measurement

A measurement is carried out when you choose the menu item **File** - **New** - **Single measurement**. As a result, you receive a window in which you can start the measurement directly.



Normally you will chose a saved method from the **Method** box. If you just installed the software, you will not find a saved method. Now push the **Graph window** button. A blank graph window will open up.



If a device is connected properly and all settings are correct, you can start a measurement by pushing the **Start** button. A measurement with basic settings (standard parameters) will be performed. You can display and change these parameters by choosing the menu item **Measurement – Parameters**. You should now see the recording of the measurement curve within the graph window. The recording finishes automatically when the number of measurements, defined in the parameter set, is reached. At any time you can stop the recording by pushing the **Cancel** button. At the end you have to save the measurement since this not happens automatically. Therefore chose **File – Save as** in the menu and save the measurement under an appropriate filename.

If you want to treat the data with other external programs, you may choose between various formats (incl. Text, Excel, XML, and Matlab).

Please make sure to save as Measurement (*.mos) as well. MultiSens can only open *.mos measurement files. The *.mos file is also the only file format, which is guaranteed to store all parameters and notes too. Most other formats only store a subset of this information to allow for easier import.

In the **Save as** window you can also chose or create another sub-directory in order to organize your data.

With the command **Options – Work directory** you can chose a sub-directory you normally use to save your data.

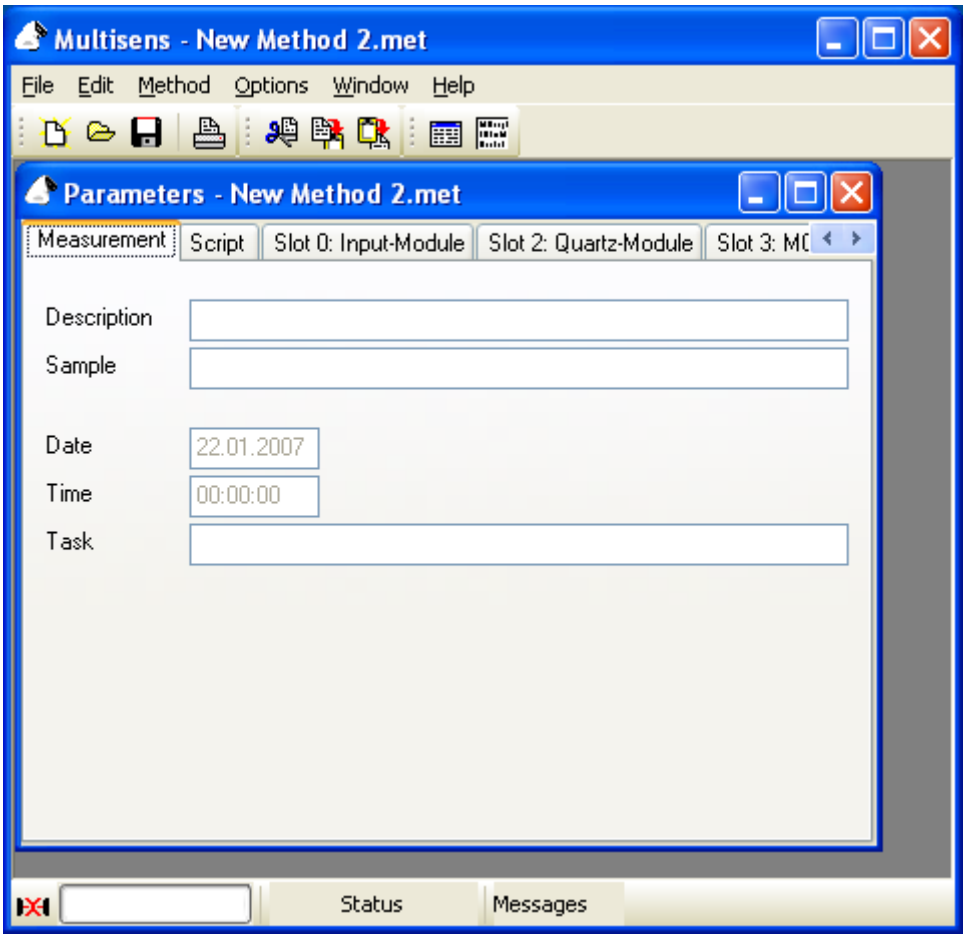
The first method

Normally you will use the same set of parameters of a device for samples of a certain class. For different classes of samples (foodstuff, plastics, textiles etc.) it may be necessary to use different methods where some parameters do not correspond to each other. If you use different settings to perform measurements you cannot compare these results directly.

A method is a file which contains all parameters for connected devices (and a combined sample preparation unit) necessary to perform a measurement. All this information is also saved and therefore documented within each individual measurement file.

Step 1: Creating a new method:

Chose **File – New – Method** in the menu. A dialog box with different tabs opens where you can adjust different settings.



Depending on the set-up of the devices a certain number of tabs is available. So don't be confused if the dialog box in your software differs from this figure in the manual. On the tab 'Measurement' you may only edit the description box. In this box a short description of the method could be introduced.

Step 2: Storing a method under a certain name:
Now insert ‚standard method' in the **Description** field.

The available parameters of a measurement will depend on your measurement setup. For this first trial we do not want to make any changes to these parameters.

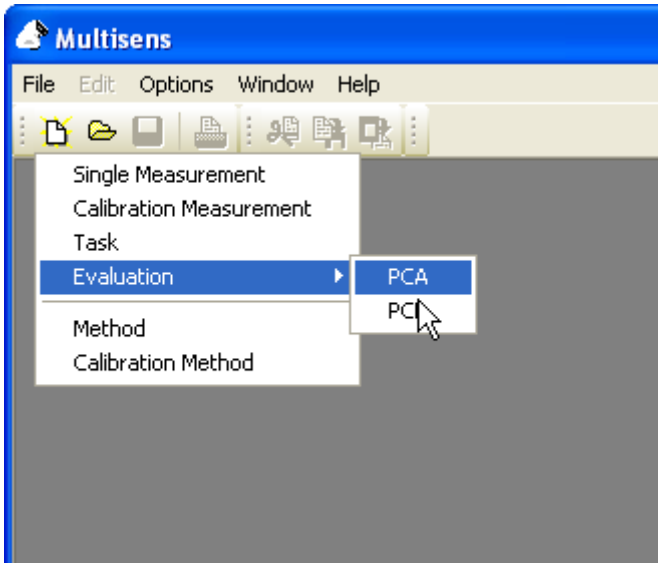
Step 3: Saving a method:
Now save the method by choosing the menu item **File – Save as**. A dialog box will open up where you can introduce the name of the method. Important! Please do not change the sub-directory of the method. Methods always have to be saved in the 'Methods' sub-directory.

Herewith you already created your first method.

The first evaluation

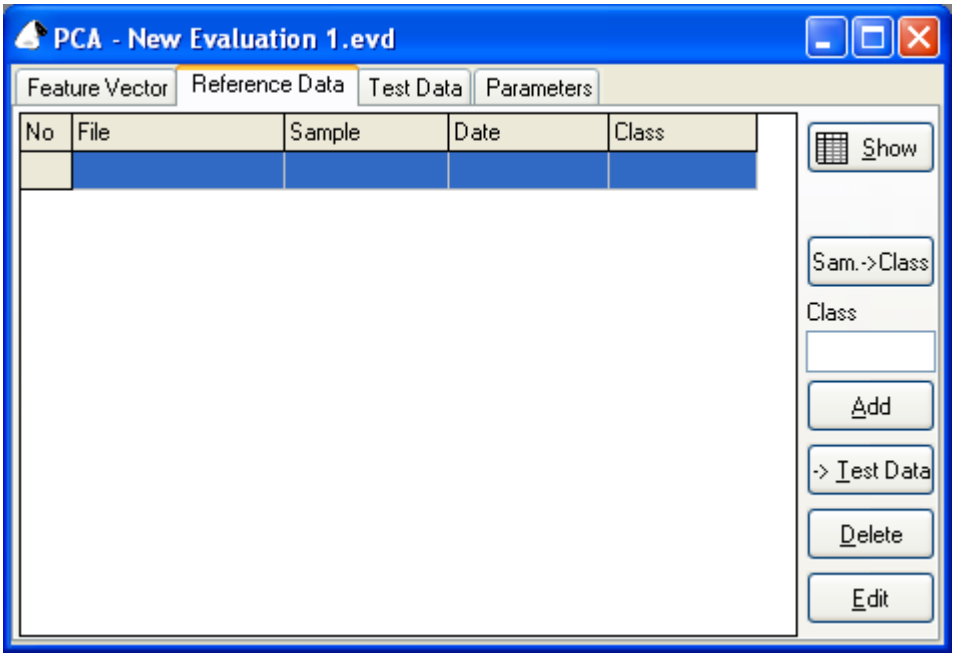
A single measurement on its own, does not provide too much information. By comparing this measurement with reference data, i.e. with measurements of known samples, the information of the new measurement can be revealed. The "Evaluation" part of the MultiSens software serves this purpose.

Step 1: Creating a new evaluation:
On this occasion we want to learn about a great relief in the MultiSens software: The icon bar. Through the icon bar you have fast access to the most important menu commands. Now click on the leftmost icon in the icon bar. A menu pops up. In this menu choose **Evaluation** and then **PCA**.



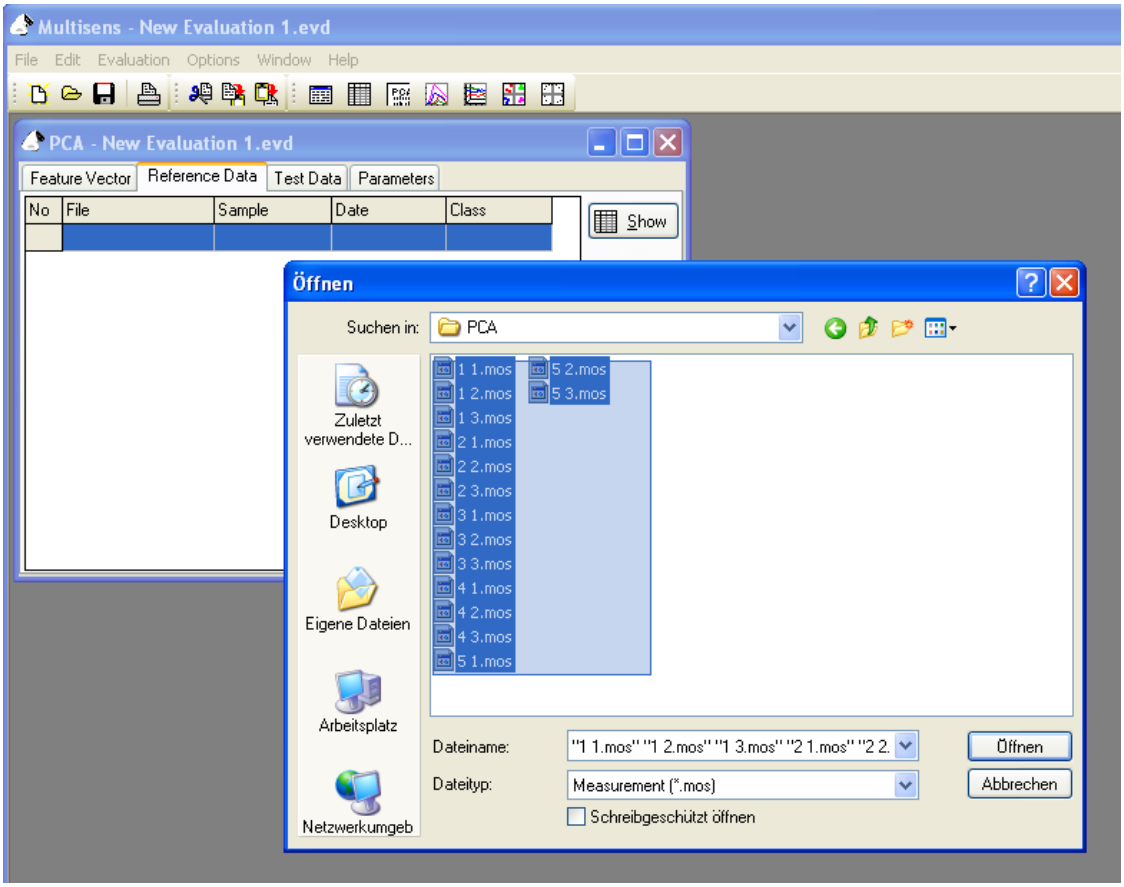
Hint: If the mouse cursor remains over an icon for a few moments without clicking, a short descriptive text will appear.

An evaluation compares several samples with each other, or with reference data. What exactly are reference data? Reference data contain those measurements that were used to build the mathematical model that is used as the framework to classify the samples. It is impossible to build a model without reference data. When creating a new evaluation, designating reference data (which must already exist at this time!) is the first step. Consequently, the corresponding page is automatically activated:



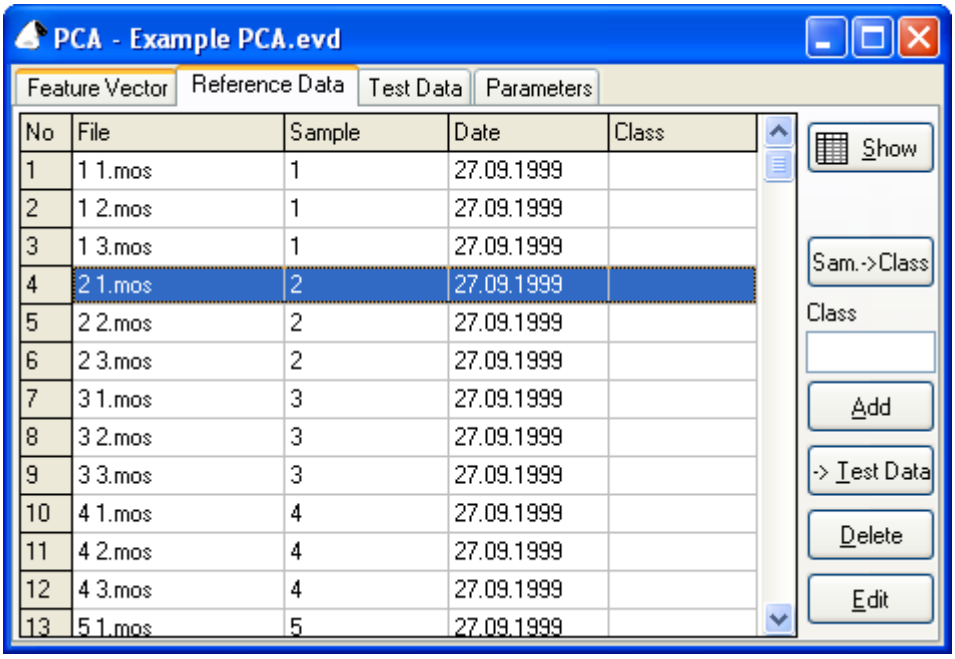
Step 2: Introducing reference data:

Click on the **Add** button. A new dialog window will appear. Change to the Examples subdirectory, and highlight all measurements. To highlight many files at once, either click-drag the mouse to draw a marquee around the desired number of file names, or highlight the first file name, then shift-click on the last file name. Then click **Open**. Please note, that while MultiSens is available only in English this Dialog will use the language of your windows installation.



Hint: You can repeat this procedure a number of times in order to add further measurements to your reference data.

Finally, the result should look similar to the example shown below. The sequence of samples is of no importance.

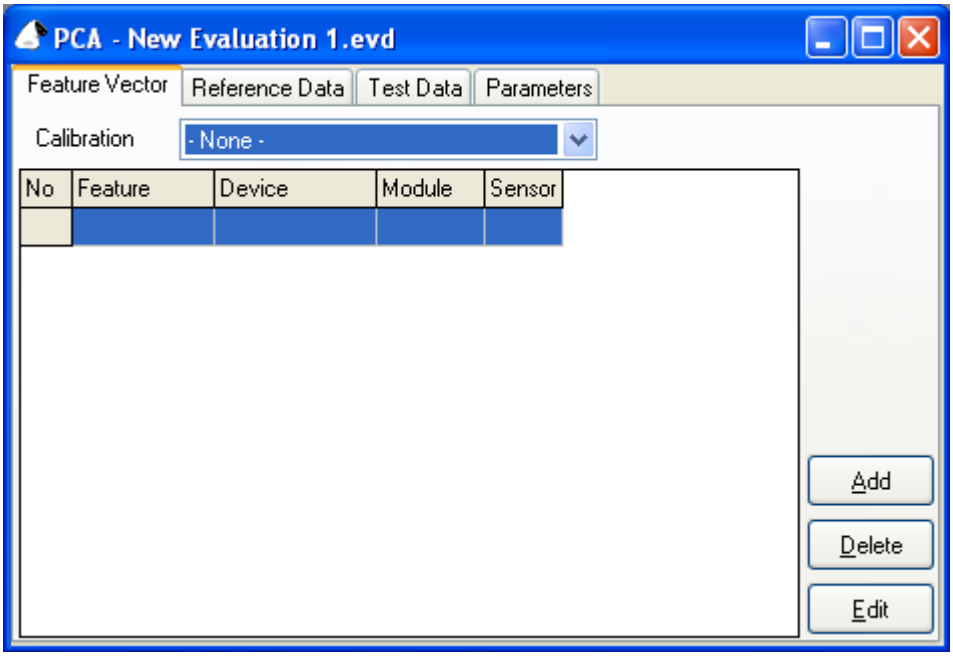


As discussed previously, each measurement contains the entire response of the sensors to one sample. Obviously, the complete response curve contains a lot of redundant information. For many types of pattern recognition algorithms, this is problematic and will in any case increase the processing time drastically. Hence, it is desirable to greatly reduce the amount of data to be processed.

This is achieved by extracting certain traits (e.g. the maximum of the response curve) from the raw signal. Such traits are called ‘features’ in the MultiSens software. The entire set of features is called the ‘feature vector’. The ‘feature vector’ comprises a number of values extracted from the sensors’ reaction to one sample.

Step 3: Generating a feature vector:

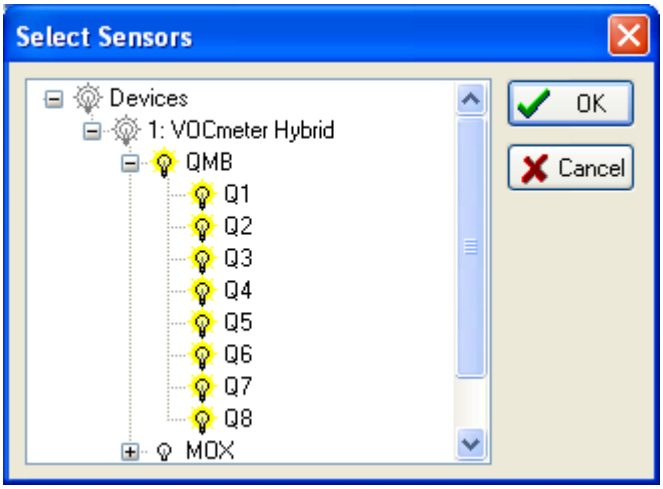
Click on the tab labeled **Feature vector**. This will bring the corresponding page to the foreground.



At this point, the feature vector does not contain any features yet. The logical next step is to first select the sensors to use, and to then define the type of feature extraction to apply. It is not necessary to use the same type of feature extraction for all sensors.

Step 4: Choosing the sensors:

Click **Add**. You will be presented with a new dialog window with a tree view of all devices in the measurements of the evaluation. Click the + sign to expand a node. Selected sensors are represented by a lit light bulb next to it. For our example, expand the module '**QMB**', and select all quartz sensors (**Q1-Q8**). Clicking on a device / module will select/deselect all contained sensors. When done, click **OK**:

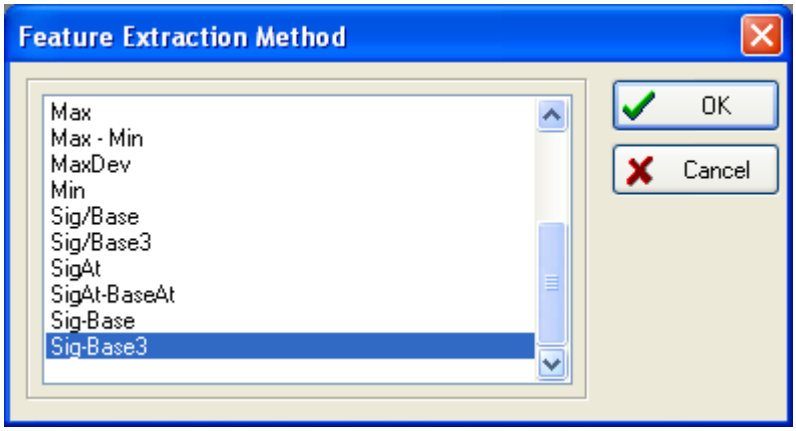


As discussed above, the next step is the choice of feature extraction method.

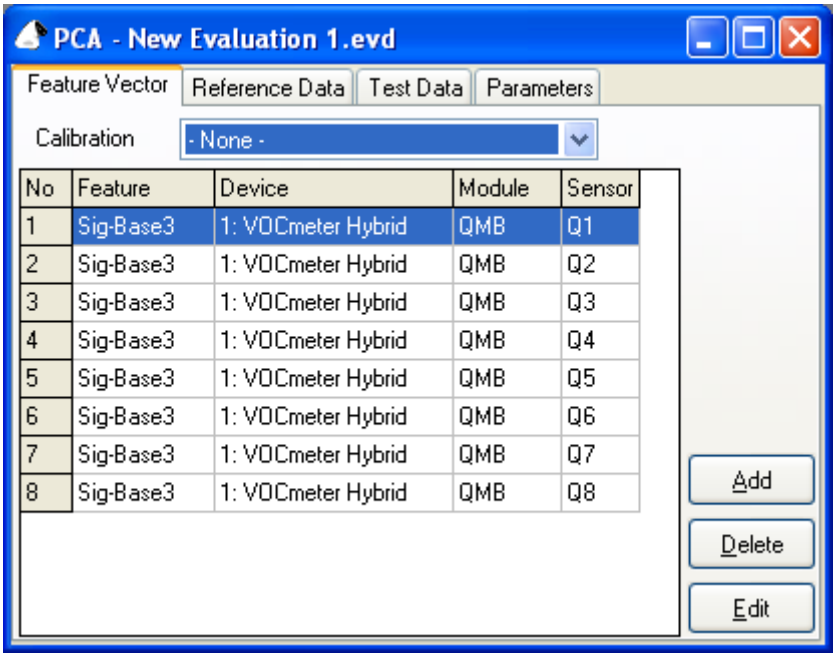
In this step we will define which value will be extracted from the sensors' response curves. The MultiSens software makes a number of different options available to you which we will discuss in more detail later. For the time being, let us just use one of the simple methods, i.e. we will just have a look at the curves' peak values. The corresponding feature extraction method is called Sig-Base3 (shorthand for "signal minus baseline averaged over 3 adjacent values").

Step 5: Choosing the feature extraction method:

In the list select **Sig-Base3** and confirm your choice by clicking **OK**:

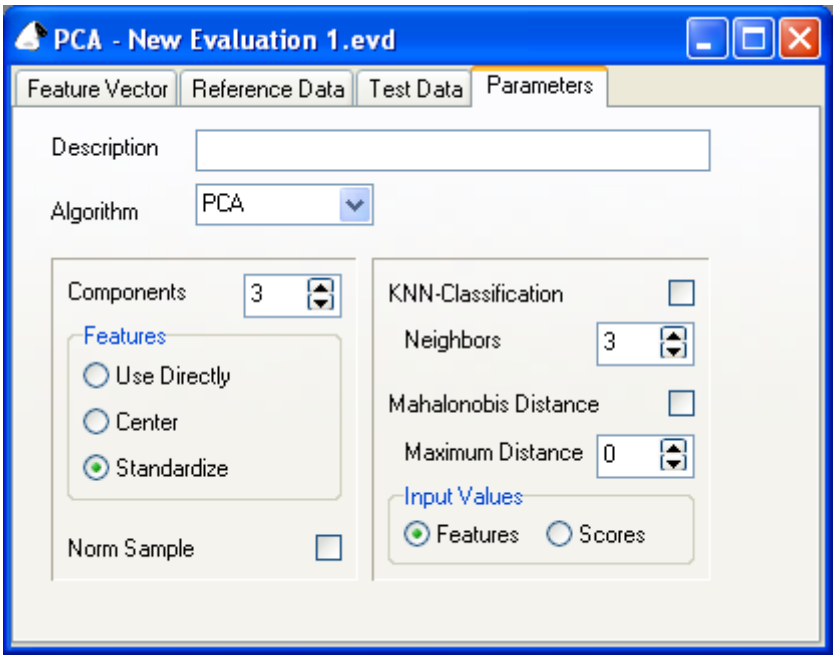


This will add eight entries to the list of features, i.e. one feature called Sig-Base3 for each sensor.



Hint: The composition of a feature vector can be chosen very liberally. It is possible to choose only one type of sensors, or even one single sensor only. Identical or different features from one sensor can be present several times in one feature vector. Obviously, the influence of one particular sensor on the final result increases with its number of appearances in the feature vector.

By now, we have defined what measurements to evaluate and how to extract one value (feature) from every QMB sensor in the measurement. Now we will select the right parameters for the evaluation. Click on the Parameter tab in the PCA window.



Step 6: Set the number of components:
On the Parameter tab set the number of **Components** to 3.

All other parameters should be left at their preset default value for the time being. The parameter **Components** determines how many principal components are calculated during the evaluation.

Before we actually perform the evaluation, let us elaborate a bit more just how the MultiSens software implements the evaluation. In this Version of the MultiSens software, Principal Component Analysis (PCA) is built in as the standard processing algorithm.

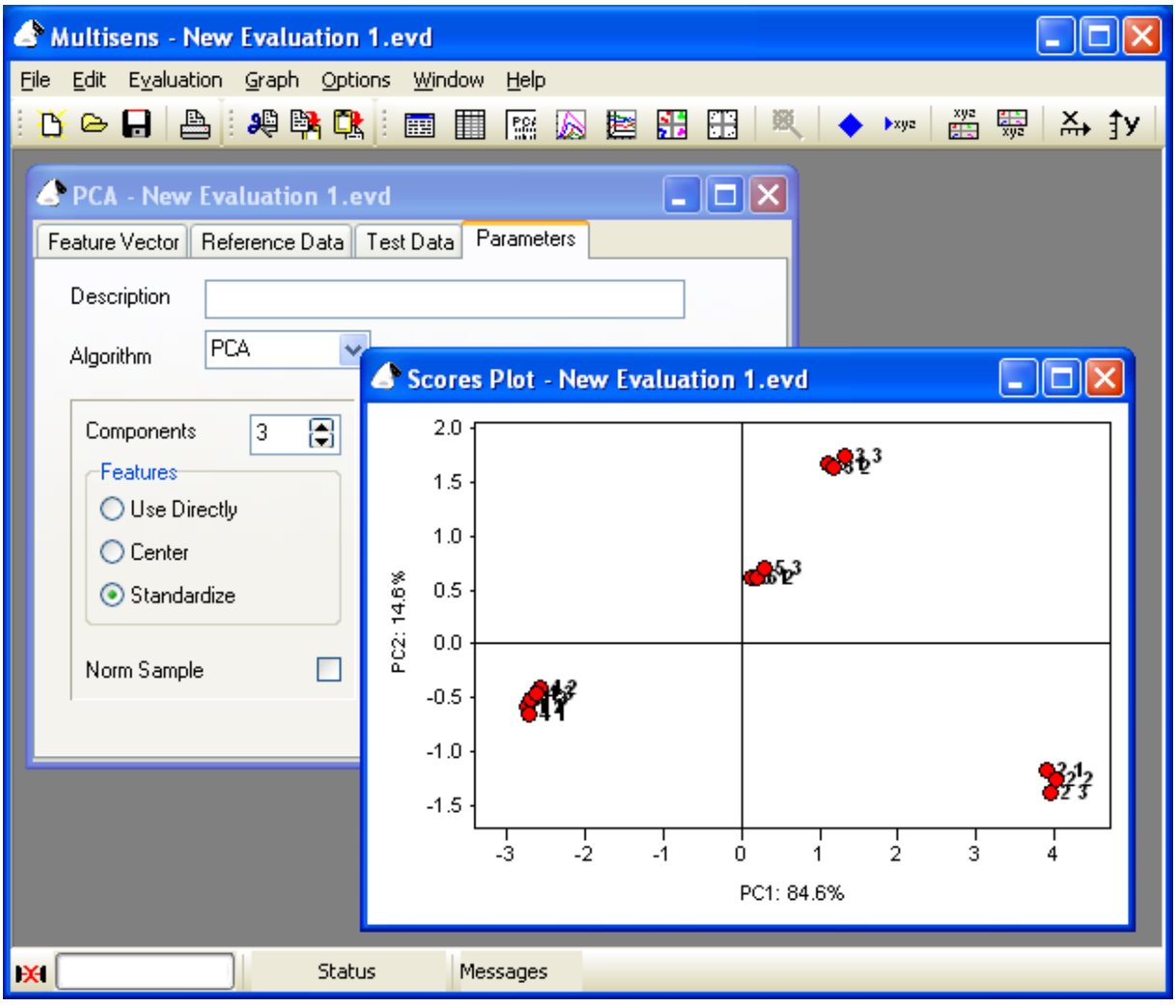
Maybe surprisingly, there is no explicit command to launch the evaluation. The MultiSens software will automatically recognize which actions are required to achieve what you mean to achieve. Hence, to have the evaluation executed, all you have to do is to request the display of the results of the PCA. The program will notice that the principal components have not yet been determined, and will automatically launch the required algorithms. All final and intermediate results will be stored in memory. This will make recalculation a lot faster because the results from a previous calculation may be re-used.

The scores plot is by far the most popular type of display for the results of a PCA. The scores plot shows the different samples with respect to two principal components (normally, the first and second PCs are shown). Similar samples turn out to be close to each other. Different samples lie further apart.

Step 7: Showing the scores plot:
From the menu, select **Evaluation – Scores plot**, or click the corresponding icon.

The program will now create a new window to contain the scores plot. Since the data have not been yet calculated, this is going to take place now. The first step is the extraction of features from the measurements. The program will briefly open each respective measurement file and perform the extraction. Once this has been completed, the principal component analysis proper will be performed. On a decently fast computer, the whole procedure will only take a few seconds.

The result should be similar to the example shown next:



Finally we need to save the evaluation.

Step 8: Saving the evaluation:
From the menu, select **File – Save as**. Like in the previous examples of saving files, select the directory that you wish to save the evaluation file to, enter a descriptive name, and click **Save**.

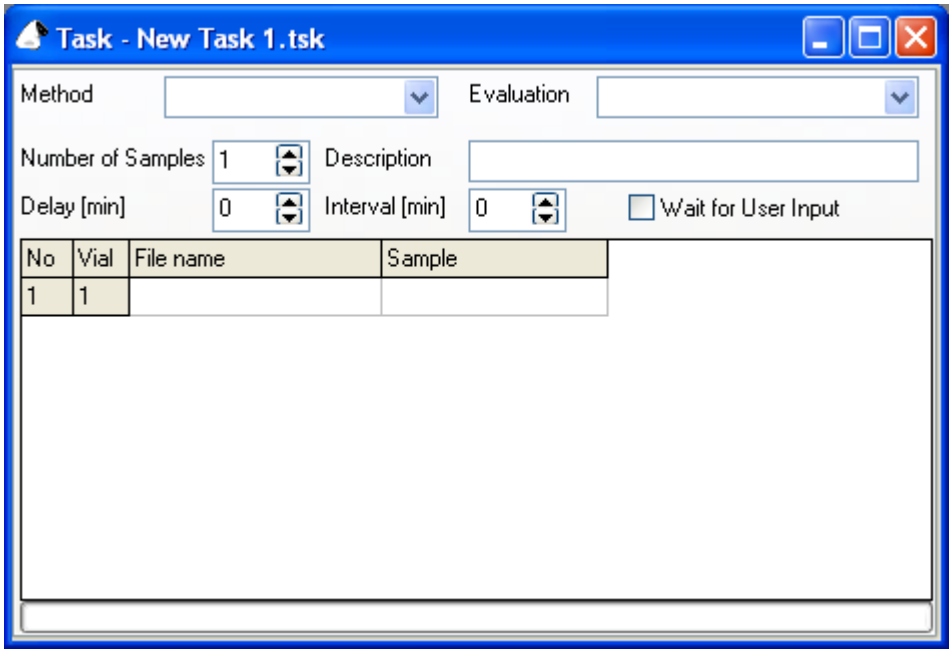
This concludes the creation of your first evaluation.

The first task

In a "real life" scenario, executing measurements one by one individually is possible, but a rather cumbersome procedure if many measurements have to be performed. In most cases you will want to have a whole series of measurements executed automatically, with no change in parameters. This is exactly the functionality provided by what we call a task in the MultiSens software. The task functionality goes together very well with the use of a headspace sampler, of course.

Step 1: Creating a new task:
To Create a new task choose **File – New – Task** from the menu.

You will now see a new window opened which allows you to make all relevant settings.



As the first step in the definition of a task, the measurement method needs to be chosen.

Step 2: Choosing a method:
Click in the list field **Method** (top left of the window), and choose the appropriate method from the list.

In this example we want to perform 3 measurements.

Step 3: Adjusting the number of samples to be measured:
Click 3 times on the upper arrow in the field **Number of samples** or write the number directly in that field using the keyboard. Notice that the table below will adapt to show the correct number of measurements, whenever the number is changed.

In the field **Description** the task can be further described:

Step 4: Describing the sample:
Enter a short descriptive text in the field **Description** (i.e. Test task).

Leave the fields **Delay**, **Interval** and **Wait for user input** unchanged.

As discussed previously, the task consists of a sequence of individual measurements. As we already know, each measurement's data are stored in a separate file. Hence, you will know have to specify the file names for the measurement files created by the task.

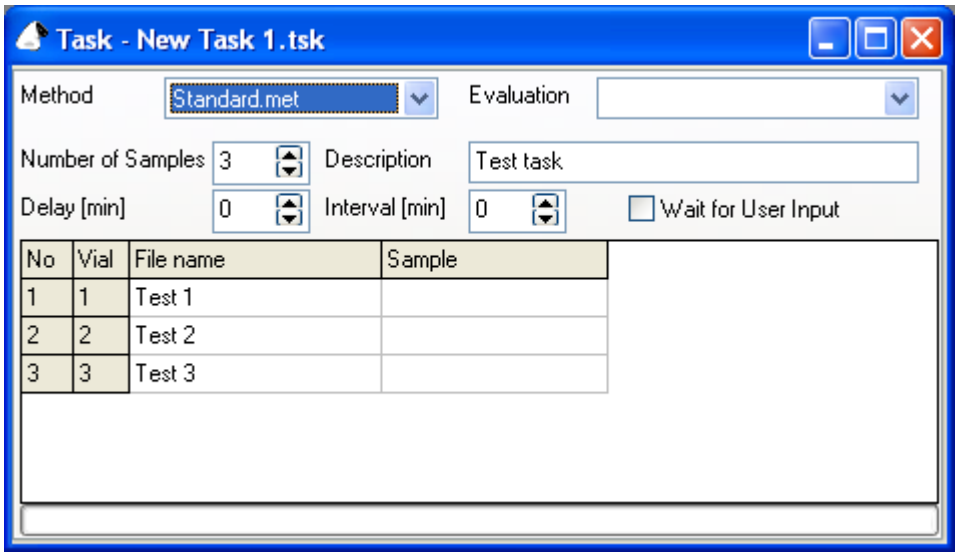
Step 5: Entering the file names:
In the table which contains one line per measurement, enter the file names now (e.g. Test_1, Test_2, etc.).

Attention:

Obviously, two measurements (samples) can not have the same file name. If you accidentally enter identical file names for two measurements, the task will not be able to execute.

For information purposes a descriptive name can be assigned to each sample. Unlike file names, sample names may be identical. As a matter of fact, you may even leave sample names blank (although in a real life situation this is not desirable).

Step 6: Introducing the sample description:
Enter a descriptive name for each sample. (i.e. ‚Test').



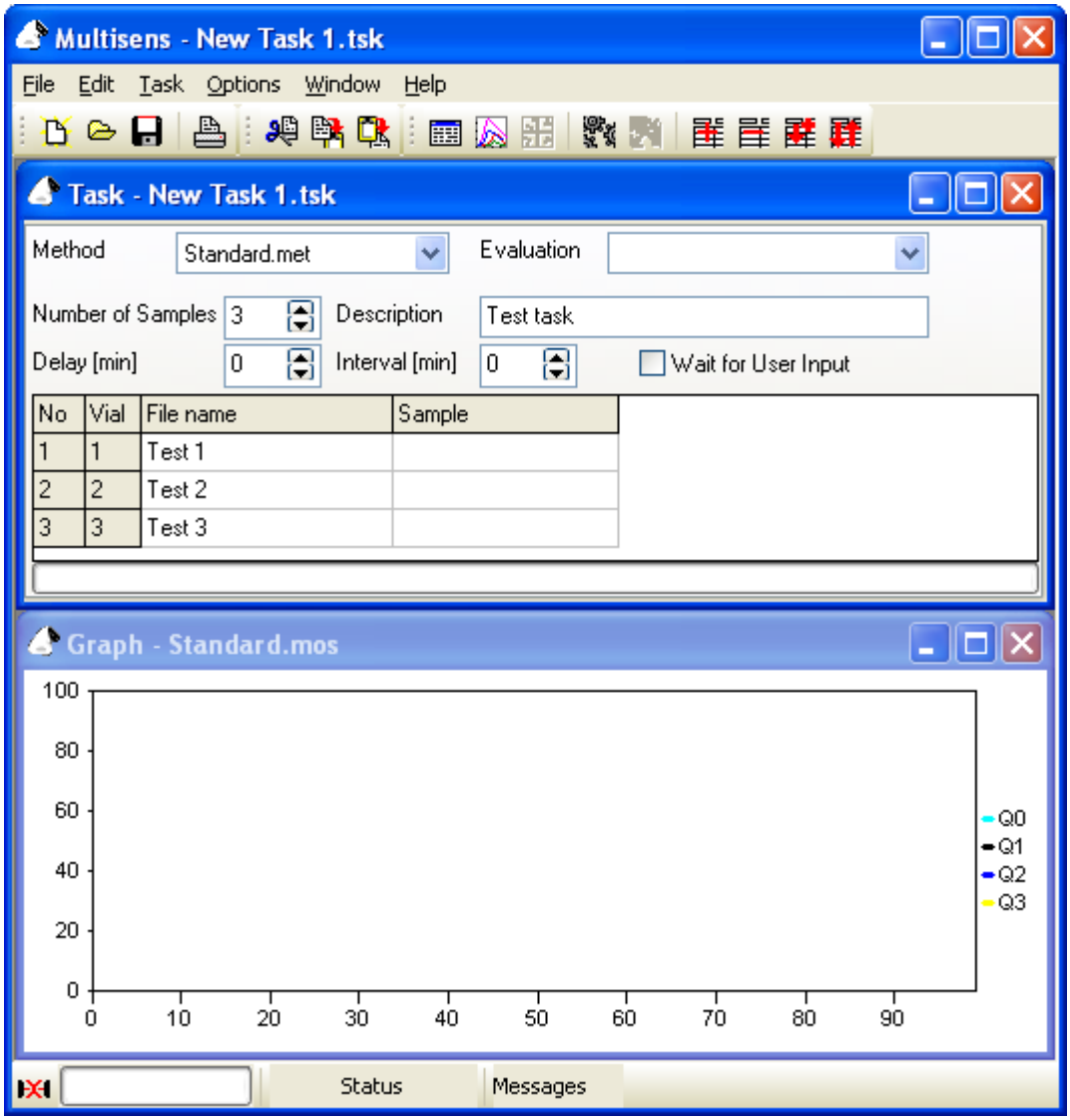
While the task is being executed you will probably want to follow the measurement's data as it is acquired.

Step 7: Opening a graph window:
In the menu choose **Task – Show measurement**.

Another window will open up, showing the measurement's data.

*Hint: Only sensors from one module can be displayed in one graph window. Which module is being displayed can be selected from the list box in the icon bar. Under the **Graph** menu entry, individual sensors can be enabled or disabled for display. If you want to watch several modules simultaneously, simply repeat the operation of opening a new graph window any number of times.*

*Hint: To reduce screen clutter, first minimize all windows that you do not whish to see during execution of the task, then select **Window – Tile Horizontally** or **Window – Tile vertically** to rearrange the remaining windows sensibly.*



Step 8: Starting the task:

Activate the Task window(The window on which you filled in all settings of the task). From the menu, now select **Task – Start**. The program will now prompt you for a file name under which the task will be stored. Enter a file name and click **Save**.

At this point, the task will be started. In the Status line of the MultiSens program you will see the number of the current sample and the total number of samples displayed in the second field from the left.

Now, simply wait for all the measurements to complete. Unlike previously, there is no need to explicitly save each measurement. The task scheduler will take care of that.

Detailed description

The basic concept of the MultiSens software

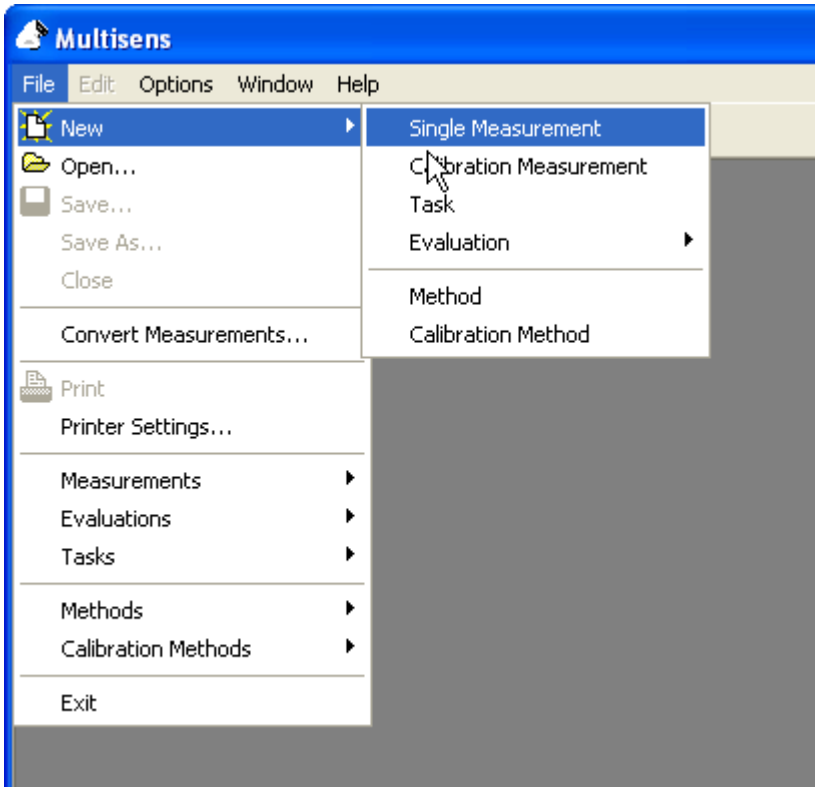
MultiSens is a single ,,all in one" program including all important features. In detail, this is control of the VOCmeter or MOSES II parameters, data acquisition, data evaluation and graphical display of raw and processed data.. Despite this multitude of functions we have focused on an easy usability. The concept of MultiSens is in line with many popular ,,file centric" windows applications. Many files can be kept open and active simultaneously. A file in conjunction with MultiSens software is a named container for data logically belonging together and hence we have MultiSens files containing measurement data (*.mos), evaluation results of different measurements (*.evd), the information on a task (*.tsk), measurement methods specifying all information that is needed to take a measurement (*.met) and a calibration methods with all information to perform a calibration measurement as well as the calibration data that has been extracted from these measurements (*.cal).

Different functions of MultiSens will be combined automatically and logically correct assigning them to the corresponding file types.

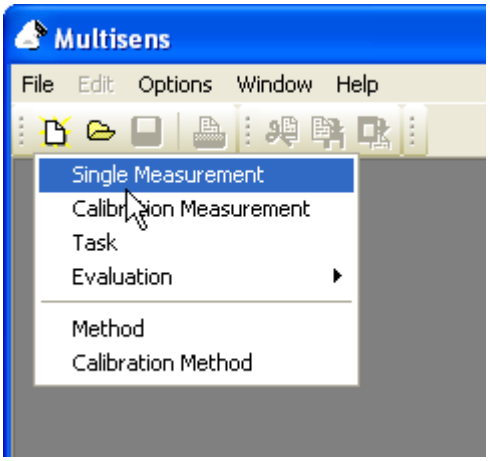
The most important command: File - New

Since MultiSens uses a file based concept, the command to create a new file, is one of the most important ones. This command can be reached in two ways:

First, by selecting the **New** submenu from the **File** menu (e.g. by pressing Alt-F followed by N),



and second, by selecting the first symbol from the left in the icon bar.



In either case you can select different functions.

The different files within MultiSens

As mentioned before, there are 5 different types of files used by the MultiSens software:

Type	Extension	Description
Measurement/Calibration measurement	*.mos	In this type of file the settings concerning a measurement as well as the raw data are saved.
Task	*.tsk	In this type of file the sequence of single measurements and their combination in an evaluation is saved.
Evaluation	*.evd	In this type of file the settings and the results of an evaluation are saved.
Method	*.met	In this type of file the protocol for a measurement is prescribed.
Calibration method	*.cal	In this type of file the selected measurements and sensors for a calibration method are determined.

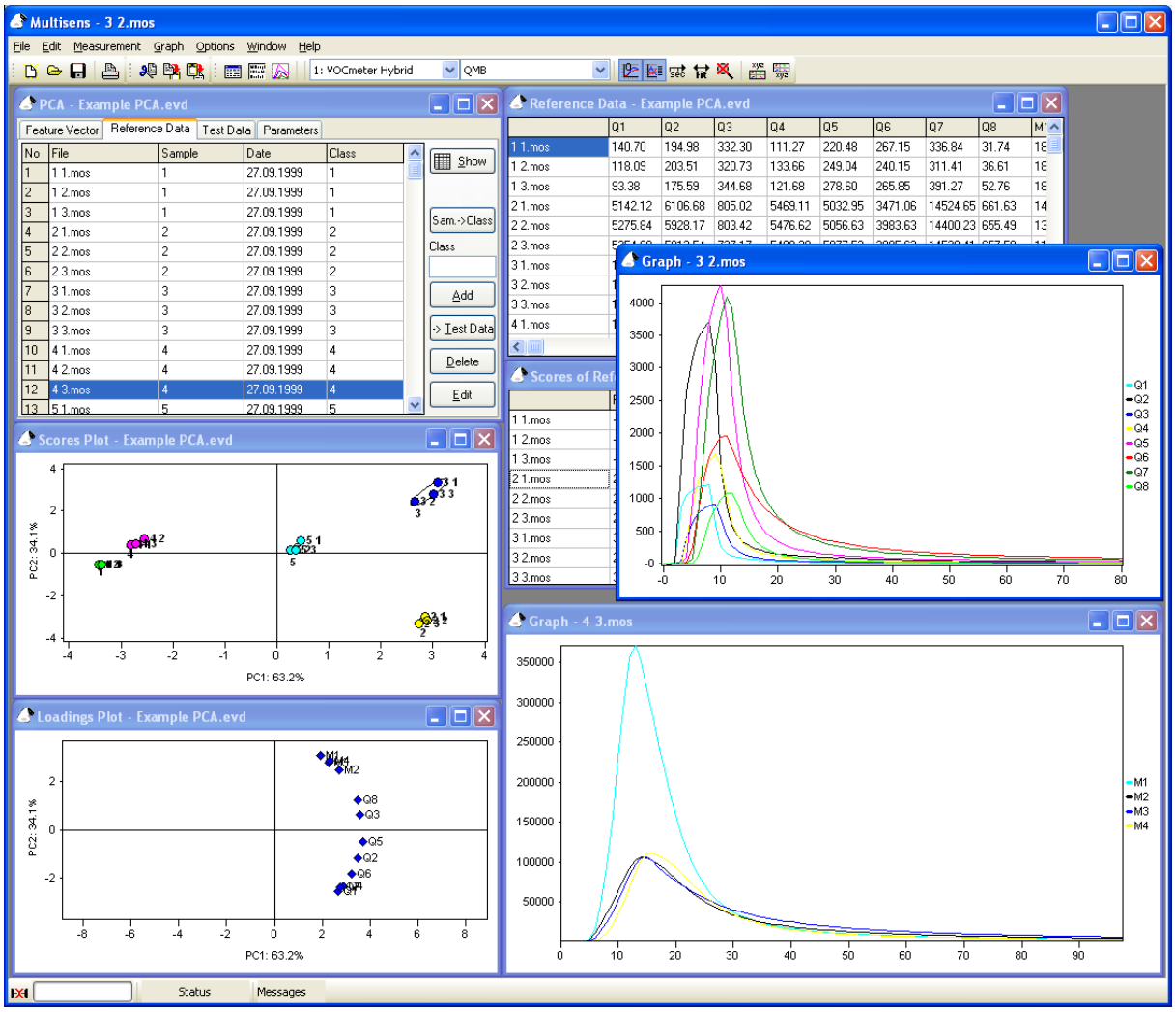
In addition to these files, MultiSens may export other files types incl. *.txt, *.xls and *.xml.

Files and windows within MultiSens

There are several possibilities to represent the contents of a file in MultiSens and to have several views of one file on the screen simultaneously in different windows. To close all windows belonging to one file, select **Close** from the **File** menu. If you have previously made any changes to the contents of the respective file, MultiSens will prompt you to confirm whether you wish to save these changes. If you reply "No", your changes will be lost. If you close one of several open windows pertaining to the same file, only the closure of the last remaining window will invoke the prompt dialogue.

MultiSens is a multiple document application. This means that you can keep several documents opened simultaneously. For example. you may want to have two measurements on the screen at the same time, making direct comparison easy. Or, you are performing an evaluation involving several measurements, and you want to revert to the raw data of one particular measurement. At any point, you may simply open the respective file without having to close what you are currently doing. However, this possibility should be used sparingly; there is a very real danger of cluttering the screen with dozens of open windows. Also, a decent monitor size (17 or more inches) is preferable for use with MultiSens.

The **Window** menu lets you change between windows, and provides several possibilities for arranging windows on the screen (e.g. **Cascade**, **Tile horziontal**, or **Tile vertical**).



The example above shows an open evaluation with some corresponding windows and two measurements represented by graphs.

The content of the menu line depends on the currently active window. Most menu commands refer directly to the active window and its file. The title bar of the active window is shown in a different color.

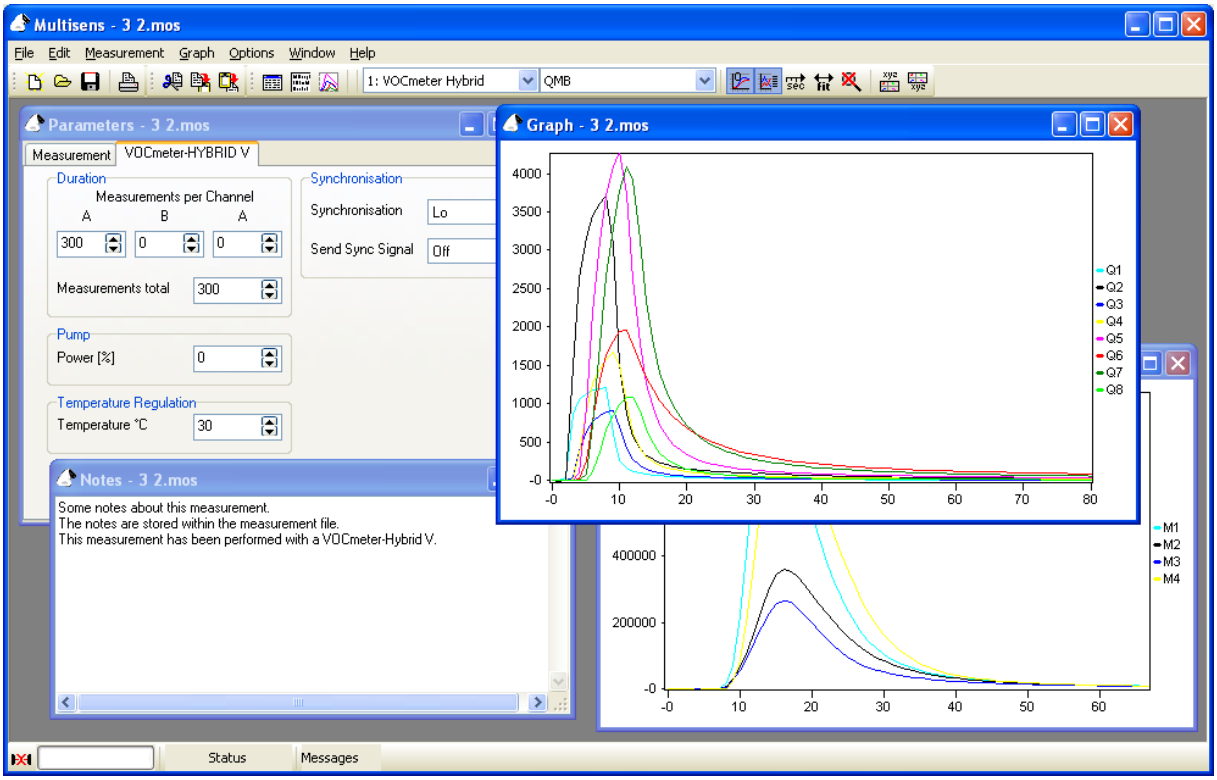
It is possible for the menu line to change its contents when you change from one window to another one (the same is true for the icon bar). In addition, some commands depend on the contents and state of a file (as an example, it is not possible to start a measurement that is currently running).

The single measurement

The most important information on how to perform a single measurement has already been supplied in chapter 2.1 and therefore it is not repeated here. For details please refer to chapter 2.1.

Graphical representation of a single measurement

For each measurement several graph windows can be opened simultaneously. To do this, select the submenu **New graph window** from the **Measurement** menu.



This kind of window shows the data from sensors of one given type. The type to be displayed can be selected using the field in the icon line.

The X axis shows the time in tick units (we will explain this later) or seconds. For the VOCmeter series, one tick usually equals to one second. For the MOSES II one tick by default equals to 1200 msec (=1.2 seconds). On many devices the measurement interval (=tick rate) can be set in the measurement method. The Y axis displays the sensors output in their respective units. The **Graph** menu offers many options for customizing the graph's appearance:

By activating **Graph - Offset subtraction** you can force all sensor curves to start at a Y value of zero. The first value of the measurement is considered the offset, and will be subtracted from all subsequent values. Depending on the type of module, offset subtraction may or may not be activated by default. In either case you can always choose manually.

By choosing **Graph - Legend** you can enable or disable the legend (list of sensor names and curve colors) on the right. By default, this is enabled.

Axes are normally scaled automatically so that all values fit in the graph frame. If you want to zoom in, simply draw a frame around your area of interest with the left mouse button depressed. To return to full-

size (unzoomed) view, double click the graph window, or click on the crossed-out magnifier icon in the icon bar, or choose **Graph - Zoom off** from the menu. This menu point is only enabled when you are currently looking at a zoomed graph.

You can also enable or disable the response curve for each sensor individually. To do this, select or deselect a sensor directly under the **Graph** menu. For each sensor such an entry has been generated automatically.

You can print the graph (as it is displayed on the screen) by selecting **File - Print** , or you may choose to copy the graph to the clipboard by selecting **Edit - Copy** . Then you could insert the graph in a word processor or another application of your choice by selecting **Edit - Paste** in that application.

Export of raw data

You can also export the sensors' raw measurement data in various file formats to process them with other applications. For this purpose, you choose the menu command **File - Save as** and select the appropriate format.

Important:

There is no way to read these exported files with MultiSens. Therefore you should always save them also as .mos file too.

The method

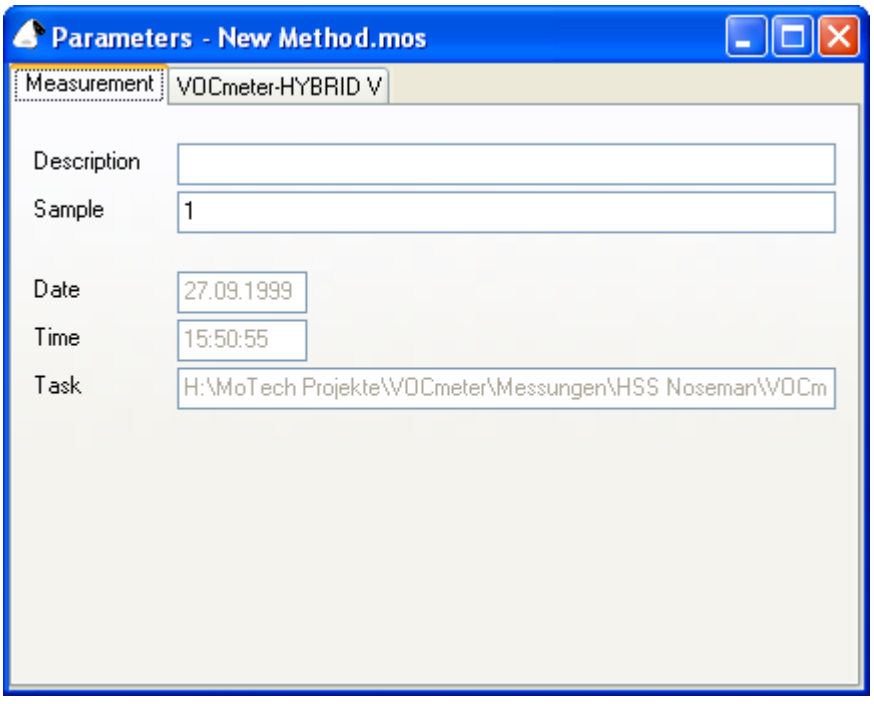
Files of type method (*.met) include all measurement setup information (parameters) for a measurement. They can be regarded as a kind of recipe for taking measurements and are stored in the 'Methods' subdirectory located in the directory where MultiSens.exe has been installed. If you have chosen the standard installation paths, the 'Methods' directory will reside in C:\Program Files\MultiSens\ ).

The parameters of a method

A measurement's parameters are displayed in one dialogue window within the MultiSens software. This window has several tabbed pages: one page for general parameters and one or several pages with parameters depending on the configuration and type(s) of devices. If you have configured to use a headspace sampler, there will be an additional page with all corresponding parameters (see chapter 0).

The page Measurement

The page named **Measurement** contains two input lines which you can use to make descriptive notes about a method. The fields **Date**, **Time** and **Task** can not be modified and will be filled in automatically when a measurement is being performed. The field **Description** can be edited when you define a method for measurements. The field **Sample** can be edited for measurements that have been performed. As this field normally is filled by the data provided in the **Task** or when a **Single measurement** is performed, a warning will appear when you try to edit **Sample**.

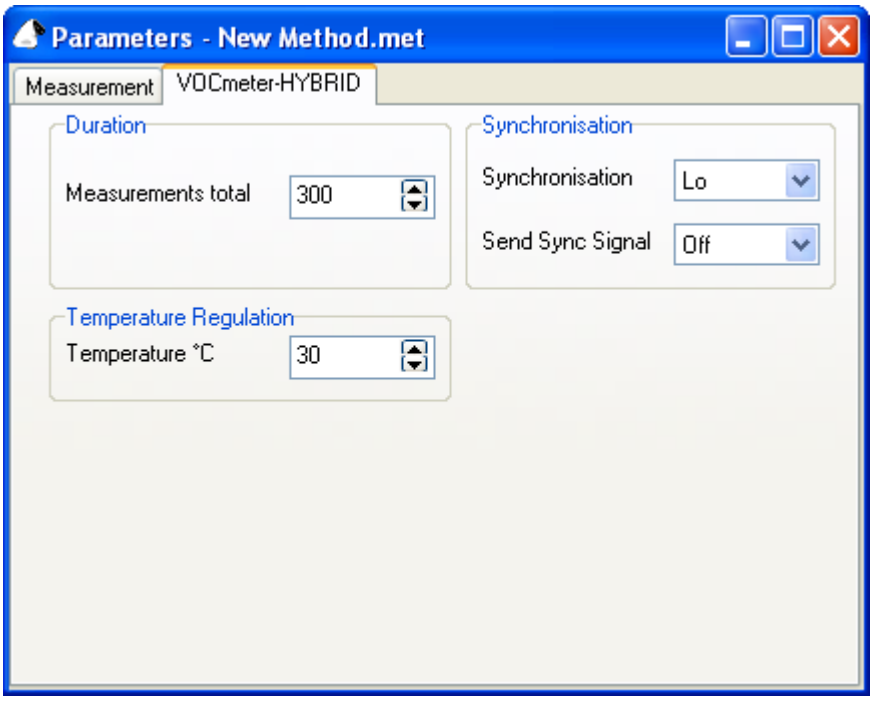


Box	Description
Description	Notes to the measurement protocol (e. g. settings of the sample preparation, type of sample, ...).
Sample	Description of the sample (this box can be blank for a method since it will be filled automatically in a task). In an evaluation the text within this box can be used to label single measurement points.
Date	Current date the measurement was performed.
Time	Current time the measurement was performed.
Task	Sequence of single measurements performed automatically.

Device dependent pages.

On these pages all device-specific parameters (e.g. concerning the timing of the measurement) are listed. You can supply additional settings in various fields which are transmitted to the attached devices before a measurement.

The device-specific page of the VOCmeter-HYBRID is shown below. First of all you can adjust the number of total measurements ('ticks'). Further, the desired temperature of the QMB measuring chamber can be set in steps of 1°C.



The area **Synchronisation** is used either for synchronisation with an external sampler or for sending a sync signal.

The input field **Synchronisation** specifies whether the VOCmeter measurement should be started immediately (**off**) or whether it has to wait until a connected device sends a corresponding ready signal.

For this purpose, the device is connected by a cable to port A of the VOCmeter.

Depending on the device, it has to be specified whether a **Hi** level or a **Lo** level signals readiness. (Please refer to the technical manual of the corresponding device for this information). For example, if you use a headspace sampler of the companies Dani or Agilent (formerly Hewlett Packard, HP 7694), it signals the injection of a sample by a **Lo** level.

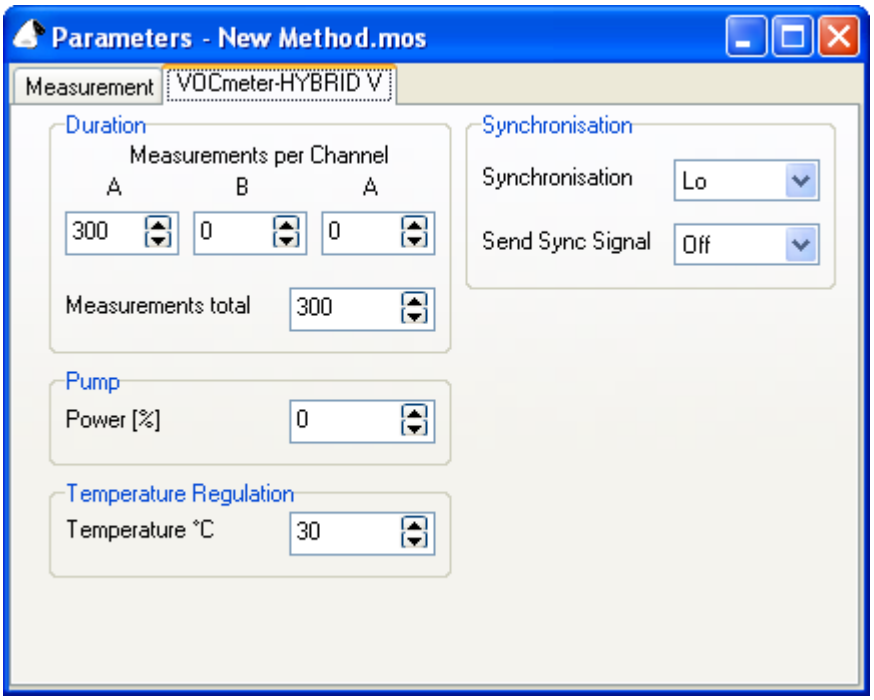
Therefore if you use one of these, set **Synchronisation** to **Lo.** So during a measurement the VOCmeter will always start at the very moment, the headspace sampler has injected a sample into the gas path.

If you choose **Send sync signal**, the VOCmeter will send a signal to an external device as soon as a measurement has been started. This can be used for example to start a sampling system or to open a valve. Here again you can specify whether a **Lo** level or a **Hi** level is used as signal.

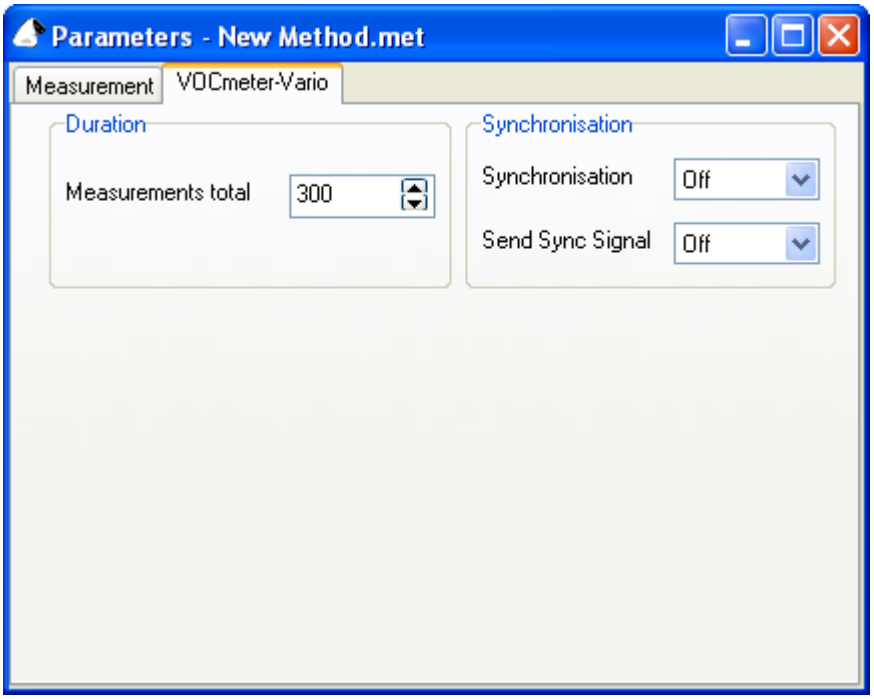
When you use both, **Synchronisation** and **Send sync signal**, the VOCmeter starts a measurement by sending a sync signal and then waits for the signal of the external device.

As a result, an external device can be started and as soon as this device has finished, the measurement will be continued.

If you use a VOCmeter-HYBRID with option V, additional parameters will be displayed on the device-specific page. As a valve and a pump are integrated, the power of the pump can be adjusted (from a minimum of 20% to a maximum of 100%) and the total number of measurements (ticks) can be selected for each input channel (A or B) individually.



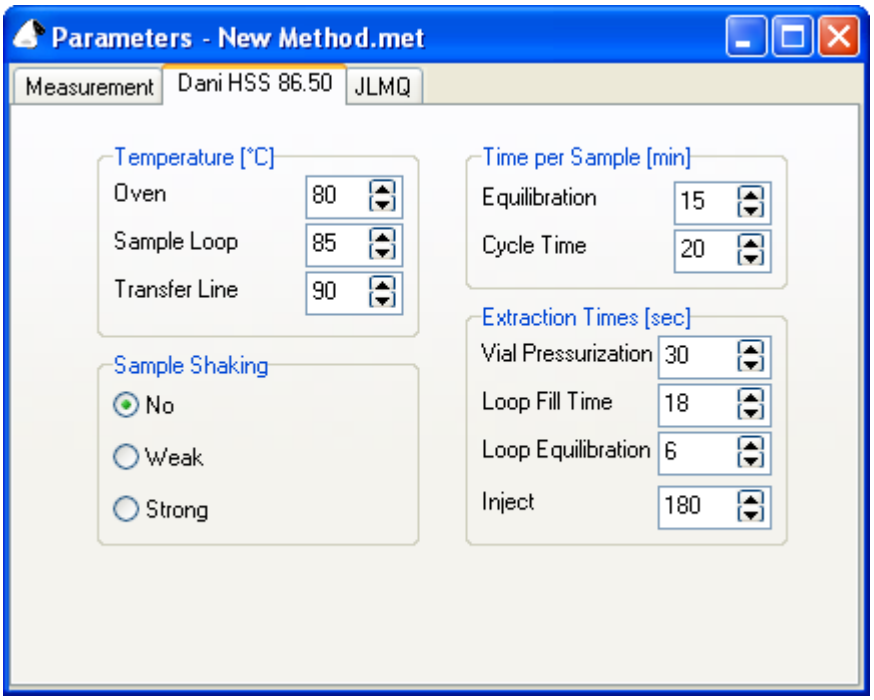
Using a VOCmeter-Vario, you only have to set the total number of measurements and possibly the desired synchronisation or the transmission of a sync signal to an external device.



During a VOCmeter measurement all sensors are recorded in fixed intervals. In MultiSens we call this time unit a 'tick'. The total number of measurements of the menu item 'Duration' corresponds to the number of 'ticks'. All times are measured by the unit 'tick'. The length of a 'tick' defaults to 1 second. The distinction between tick and second was introduced since MultiSens software is used for variety of different systems with possibly different time bases (e.g. MOSES II).

Parameters of the headspace autosampler

An additional page will be displayed after you have selected a headspace autosampler using the menu item **Options – Sampling**.



Parameters on this page concern temperatures (**Oven, Sample loop, Transfer line**), times (**Equilibration**, **Cycle time**, **Vial Pressurization**, **Loop fill time**, **Loop equilibration**, **Inject**) and the applied sample shaking (no, weak, strong).

These parameters can be transmitted to the autosampler automatically by the MultiSens software. However, up to now, this feature only works with the Dani 86.50 autosampler.

Important:

To ensure that the VOCmeter waits for the sampler's sync signal at the beginning of a measurement, the connecting cable has to be plugged in correctly and the field **Synchronisation** on the VOCmeter parameter page has to be set to **Lo**.

Calibration method and calibration measurements

The theoretical basis of calibration has already been addressed in the VOCmeter / MOSES II manual. At this point, the practical procedure for creating a calibration method will illustrated. Calibration methods specify measurement conditions and how (i.e. by means of which algorithm) the sensor data is adapted.

After the calibration method has been created, calibration measurements can be made on the basis of this method. These measurements are saved as tables within the calibration method.

If an evaluation is now carried out, one can select the calibration method that is used to adapt sensor values.

There is no fixed recalibration included in the software that has to be used for recalibration of subsequent measurements. Calibration data and measurement data is kept completely independent and is only associated with each other during an evaluation.

This somewhat complex procedure has the advantage, that different calibration strategies can be applied and compared to each other during an evaluation.

For example, if one finds that a calibration measurement was erroneous, one can remove this individual calibration measurement of the calibration method's table without all measurements carried out after the erroneous calibration measurement becoming invalid.

Algorithms available up to now, use the first calibration measurement of the calibration method (or if you select the corresponding option, the mean value of the calibration measurements of the first day belonging to this calibration method). This means that the adaptation of subsequent measurements is computed in such a way that they have values identical or close to the reference.

In order to adjust two devices, both devices must employ the same reference. This can be achieved by taking a calibration measurement (or several within one day) using one device and including this measurement into the calibration method's table of all other devices that have be adjusted.

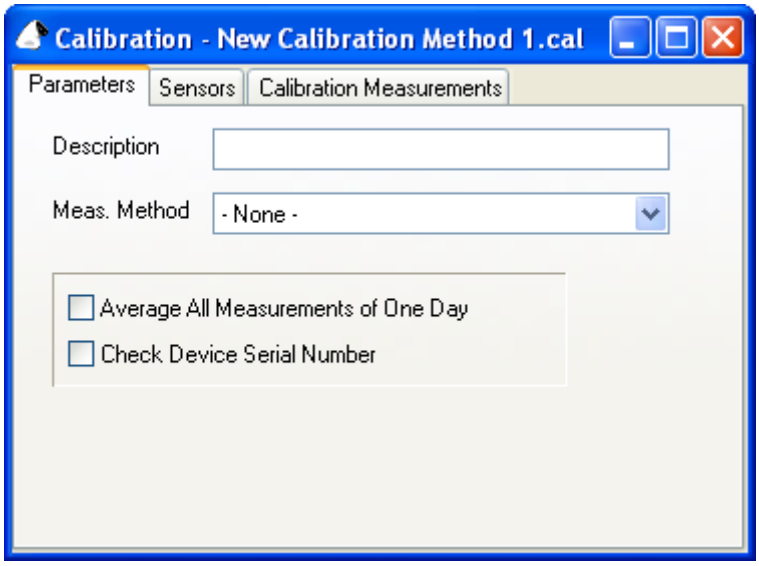
Before performing a calibration measurement it is necessary to generate a calibration method. This is closely related to the generation of an ordinary measurement as discussed in chapter 0.

Since the calibration is an important item the generation of a calibration method will be described in detail:

The first step is to select **File - New – Calibration method**:

A window with different option appears. On the first page **Parameters** the description field is used to enter a detailed description text for the method

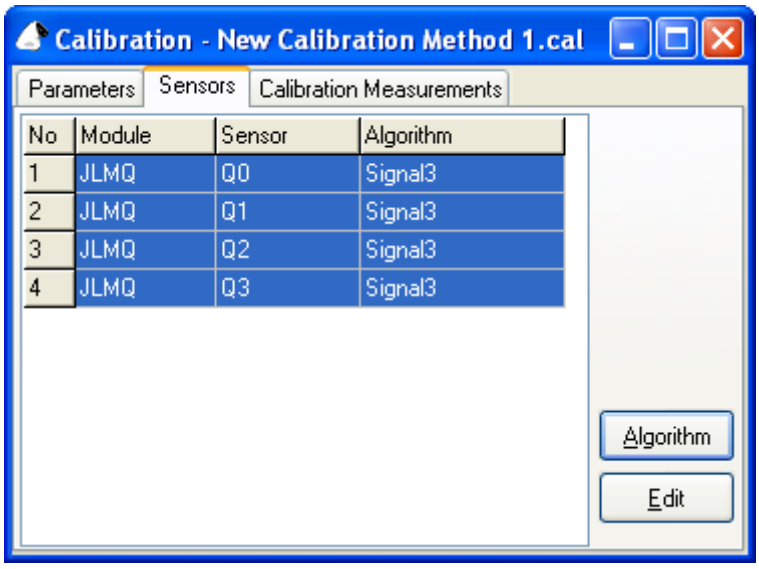
The second field **Meas. method** is used to select an already generated measurement method as basis for the calibration method. As usual the measurement methods are located in the Methods directory of the software.



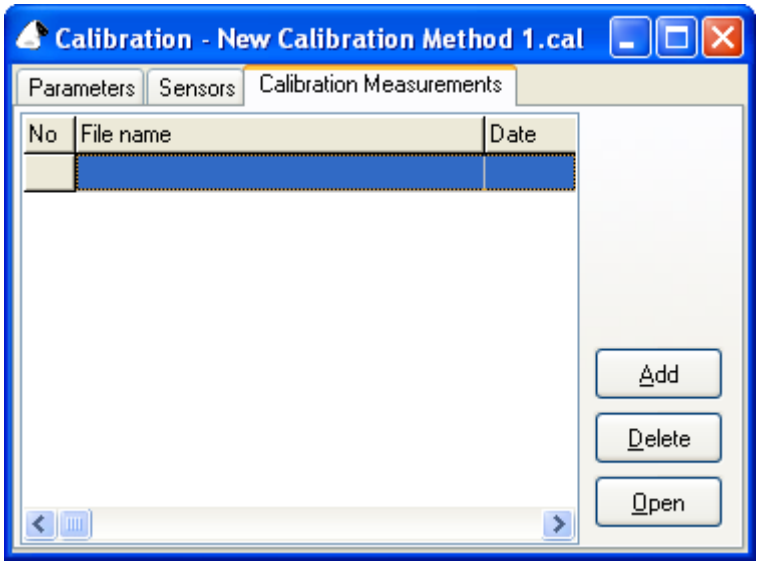
If the option **Average all measurements of one day** is selected, all calibration measurements of the respective day are used for calculating the average value which will be subsequently used to calibrate at this day.

If the tick box is not selected, the calibration measurement will be used which is the last one before the respective measurement to be calibrated.

The second page **Sensors** shows all available measurement signals. The column **Algorithm** describes the technique of signal generation which is comparable to the selection of features of an ordinary evaluation. In the picture below, the Algorithm Signal3 has been selected by pressing the **Algorithm** Button. The Algorithm Signal3 corresponds to the feature Sig-Base3.



The third page **Calibration measurements** shows a table of all performed calibration measurements in chronological order. Shown in the example Standard1 to Standard3. The algorithm is using the first calibration measurement (No. 1, first line) as a reference point. All subsequent calibration measurements are referring to this first calibration.



As usual **Add** and **Delete** are used for adding or deleting measurements to or from the list. **Open** opens a marked measurement.

Example files Standard1.mos to Standard3.mos are regular VOC-meter measurements which were manually added to the list. Using the automatic calibration the filenames are generated automatically. This is done according to the following scheme: As an example the file „new calibration method 1.cal“ is selected:

Let’s assume the scenario consists of 2 conditioning measurements and 3 calibration measurements (the meaning is described below). In the list the following files will show up (top down):

„new calibration method 1X.mos“ where X is a number from 1 to 3. This represents the number of calibration measurements. Before the following files were generated during the conditioning phase: „new calibration method 1XCY.mos“, where X is 1, because it is created before the first calibration measurement named „ new calibration method 11.mos“ and Y is 1 and 2 since exactly two conditioning measurements are performed. Conditioning data is not used and therefore not displayed in the above shown list.

Assuming a second calibration campaign with again 2 conditioning measurements and 3 calibration measurements will generate following files (in chronological order):

„new calibration method 14C1.mos“,

„new calibration method 14C2.mos“,

„new calibration method 14.mos“,

„new calibration method 15.mos“,

„new calibration method 16.mos“.

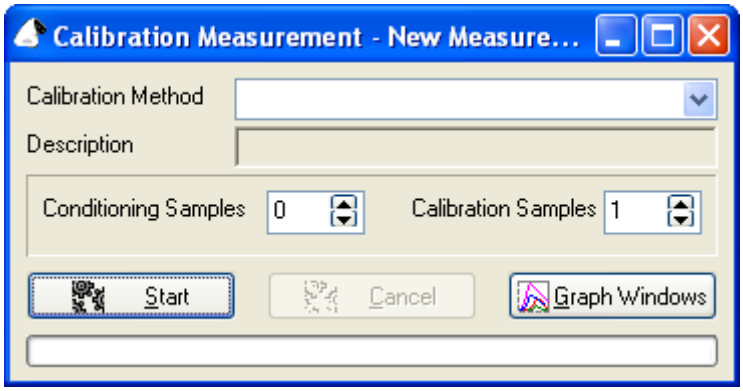
This system will be the basis for further calibration campaigns.

The background and mechanism of this system will be given in the following:

After the definition of all parameters the calibration method here „new calibration method 1“ will be stored in the directory Calib of the software. The filename can be selected by the user as usual.

After the definition of the calibration method and saving the real calibration measurements can be started.

The calibration measurement is selected by **File - New – Calibration measurement.** The following window will appear:



The field **Calibration method** allows to select (user) predefined calibration methods. The field **Conditioning samples** determines the number of samples to be used for the conditioning of the system (is equal to the number of headspace vials in the headspace sampler). The purpose is to ‚adjust the sensors' (conditioning). These measurements are not used for the subsequent calculation.

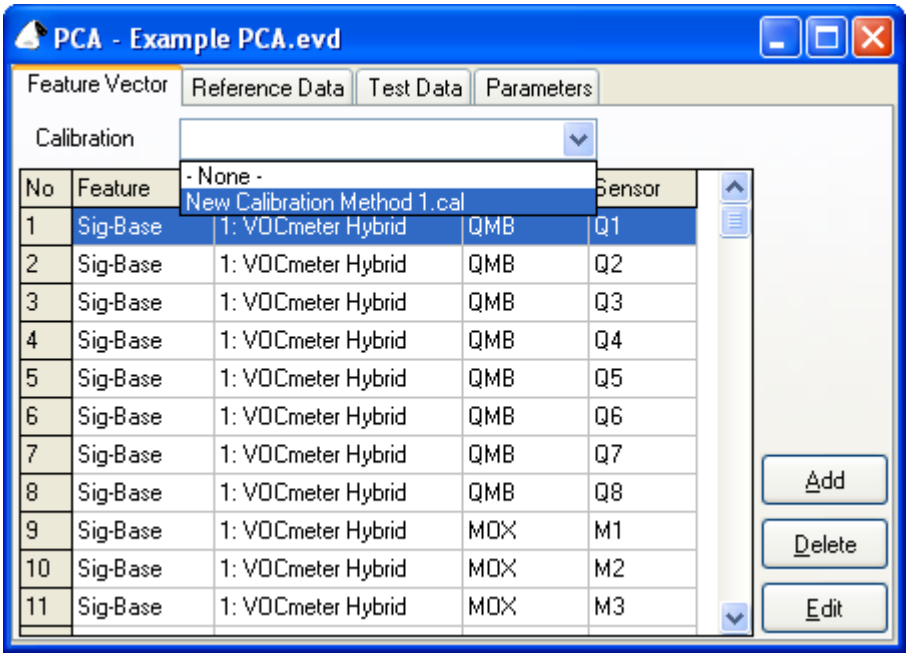
Field **Calibration samples** determines the number of calibration measurements to be run. Calibration measurements are directly started after conditioning measurements.

The frequency of running such calibration campaigns consisting of conditioning and calibration measurements is totally application dependent. It may also determine the precision of the measurements. For some application one calibration campaign per day might be necessary, most application however will need less frequent recalibration (every week or even every month).

Is the option **Average all measurements of one day** in the calibration method selected all calibration measurements of the respective day will be used to calculate the average value. Measurements on this day will be calibrated by this mean value.

If this option is not selected measurements will be calibrated by the calibration measurement which is the direct predecessor in time. If several calibration measurements are performed in a sequence, only the last of those will be used in fact for the calibration. Several calibration measurements are in this case less useful.

Such a generated calibration method will be used in an evaluation by selecting on the first page **Feature vector** the field **Calibration** and entering the respective calibration method.



All calculations in the evaluation are now using the calibration data automatically. All necessary recalculations are instantaneously done. Since all measurement files in the evaluation are reopened for this purpose the process may require some time. If an evaluation is opened the respective calibration method is checked for new calibration measurements and the data of the evaluation is automatically adjusted. After the evaluation has been opened the calibration method is not checked for new data. This will be done during the reopening the next time.

The task

Many applications require large amounts of samples to be measured. This can be easily realized by use of commercially available sample uptake systems e.g. headspace sampler, purge-and-trap systems, thermodesorption systems etc. These systems allow an automatic gas sample uptake and preconditioning. The MultiSens software integrates a feature which allows to set-up an automatic measurement mode. Every sample delivered by the sample uptake system will be measured and saved in a file. The file name can be configured individually by the operator.

Run measurements automatically

A new task is created by the menu command **File - New - Task**. The settings for the new task can be done in the new window.

First of all a method should be chosen which contains all the parameter of the single measurement. This method must be defined before creating a task and must be saved in the folder “Methods”. The box **Method** (upper left corner in the window) presents a list of all methods saved in the folder “methods”.

The box **Evaluation** allows to choose an automatic and on-line data evaluation. Chapter 0 describes the details of this function.

The box **Description** allows to add a text containing e.g. specifications of the sample preparation or a description of the purpose of the measurements.

The box **Number of samples** represents the number of samples which will be measured automatically. The number of rows in the table below corresponds to this value. Each row represents a single sample and measurement. If the number is increased new rows will be added at the end of the table, if the number of samples is reduced, the last surplus rows are deleted. If you want to delete or add samples within the existing task use the menu command **Edit - Delete Sample** and **Edit - Insert Samples**. Both commands appear additionally in the corresponding icon bar.

A task can be synchronized with the sample uptake system by a direct connection (using a dedicated cable, see the VOCmeter / MOSES II manual). The sample uptake system must therefore be equipped with a remote control port.

The boxes **Delay** and **Interval** allow to synchronize the VOCmeter / MOSES II if a hardware connection cannot be established or a user defined timing shall be used. **Delay** represents the time between start of the task and start of the first measurement (e.g. the time which is necessary to thermostate the sample uptake system after start-up) **Interval** describes the time between two measurements (which is necessary e.g. to equilibrate the temperature of the new sample in the sample uptake system or to stabilize the baseline of the sensors). Both values are to be specified in minutes. (Interval is equivalent to the parameter cycle time on a headspace sampler and defines the rate at which measurements are performed.)

The table consists of a variable number of columns. The first two columns denote the number of the measurement **No** and the number of the sample container **Vial** in the sample uptake system. Both columns are filled in automatically. The column **Filename** must be filled in by the operator. The measurement will be stored using this filename. Each sample needs therefore a different filename, the operating system Windows 9X/NT ™ limits the use of several characters. A more precise description of the sample can be added in the column **Sample**. The text typed into this cell is transferred to the field **Sample** in the measurement file (*.mos).

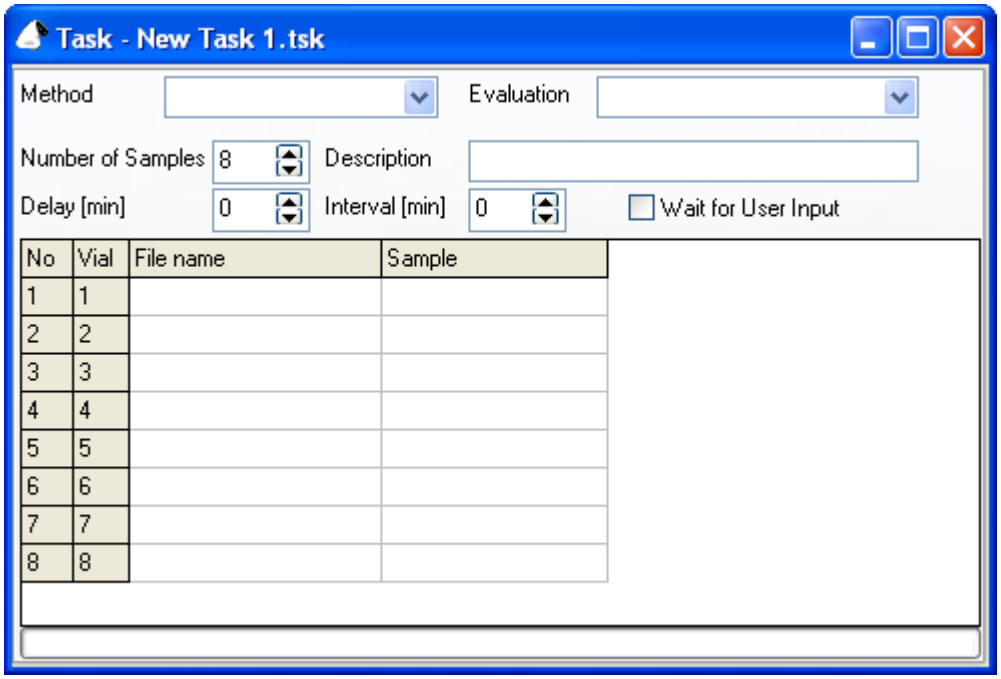
Hint: The filename or the sample description can be used to label samples within the data evaluation figures. Short filenames or abbreviated descriptions help to keep clearness of the figure.

*Hint: The command **Edit – Fill samples automatically** allows to generate filenames automatically. All empty filename cells are filled out. The filename of this samples is composed out of the filename*

given in the cell above all empty cells and an additional ascending number. The filename will be added to the corresponding column „sample" except for cells that already contain a text.

The field **Evaluation** determines (if and which kind of evaluation is selected) the number and type of parameters in additional columns. The column **Evaluate** selects the samples to be evaluated. The samples measured within this task are always evaluated as test data. Further columns will show the results of the evaluation generated during the task. Assuming the evaluation to be a PCA and within the PCA KNN classification is activated generates an additional column giving the classification results. In a PCR the result in the additional column is the predicted value.

Hint: To be able to select an evaluation within a task the evaluation has to be stored in the Methods subdirectory of the software.



Field	Description
Measurement	Measurement protocol which defines the recording parameters.
Evaluation	Basic settings for the evaluation to be performed.
Number of samples	Number of single measurements to be performed.
Description	Notes to the task (e. g. settings of the sample preparation, type of sample, ...). The text within this box is also transferred to the description of the automatically performed evaluation.
Delay	Delay time after which the measurement starts.
Interval	Time between two single measurements.
Wait for user input	If activated a dialog window with a prompt will appear before a measurement is performed.

Column	Description
No	Number of the measurement.
Vial	Sample container (vial) or number of the sample in the sampling system.

Filename	Name of the saved measurement file.
Sample	Description of the sample (transferred into the ‚sample' box of the measurement file).
Evaluate	Introduction of the measurement into the test data set of the evaluation.
Classification / Value	Class the sample belongs to (PCA) or predicted value (PCR).

Using the command **Task - Start** is starting the task, using the command **Task - Stop** terminates the task before regularly ended. This requires of course the task window to be the active one.

Right after starting the task, a window will be appear that allows to save the task. Within this window it's possible to change the directory as well as generating a new one. Running the task generates as reported above for each individual sample a file with a filename given in the table. The files are stored in the same directory like the task.

Hint: Saving the task in an individual directory (or in a directory with related measurements/tasks) allows a quick identification of the measurement files. Reason for this is as already stated that the measurement files are stored in the directory of the task. Using the system for a given time generates a large number of data files which should not be stored in the program directory of the MultiSens software neither in the Methods directory.

Using the command **Task – Show measurement** allows to generate several graphic windows displaying in parallel even during the task (see 0).

Running measurements and evaluations automatically

The software is generating automatically an evaluation upon start of the task if during the definition of this task an evaluation method is entered in the field **Evaluation**. The new evaluation will have the same filename as the task (the extension is of course different). The new evaluation is based upon the evaluation method selected by the field ‚Evaluation' (= evaluation file, located in the Methods directory of the software). In consequence the new evaluation contains all parameters as well as all reference and test data of the evaluation method. Upon completion of a measurement in the task the measurement will be automatically introduced into the evaluation as test data.

*Hint: The content of the field **Description** in the task will be automatically transferred to the field **Description** in the evaluation. This field can be used in the title and subscript in the graphics of the evaluation and therefore also as headline of the graphics (using the macro ‚{Description}').*

Using the command **Task – Show evaluation** is showing the default graphic (e.g. scores plot in the case of PCA) of the automatically generated evaluation. During the run of a task the graphic is updated automatically as soon as a new measurement is finished and saved.

The evaluation

An evaluation is used to compare measurements with each other, and/or to classify new measurements according to previously recorded measurements.

As you will probably guess by now, creating a new evaluation is not much different from the other "creation" procedures discussed previously, i.e. you do **File – New – Evaluation**. Instead of always starting from scratch you may also choose to load an existing evaluation, modify it, and save it under a different name. Very much like measurements that can turn into methods by storing them in one specific directory, an evaluation can become a "template" for others by storing it in the Methods subdirectory (underneath the directory where the main application MultiSens resides). This way, an evaluation can be included in a task to achieve ultimate automation.

The basic procedure

MultiSens-Software has a **P**rincipal **C**omponent **A**nalysis (PCA) and optional a **P**rincipal **C**omponent **R**egression (PCR) built in. These algorithms have the striking advantage of being relatively intuitive and easy to use. There is only a limited number of parameters to "tweak", and the result is ready for immediate interpretation. PCA is a fast algorithm that can be executed in real time on a decently fast computer. MultiSens makes good use of this property by invoking PCA recalculations automatically as soon as any parameters have been modified or any data are added or removed. You never have to explicitly request a recalculation-there isn't even a command to achieve that. The program will recognize automatically what needs to be done.

Normally you will want to start evaluation work flow by defining which measurements you want to include. Then, define a few basic parameters (definition of the feature vector). You will want to view the result immediately as a scores (scatter) plot. In addition you may want to open further windows containing the features matrix, a loadings plot, etc.

All these windows pertain to one single file though. They just show different views. Changes made in any one of these windows will immediately proliferate to all other windows. Hence, you will hopefully soon find this an inspiring environment that will encourage you to "play" with your data in many different ways. Furthermore it is possible to load several evaluations simultaneously and compare the different results.

Reference data

To start an evaluation you will need reference data. Those data that are used to construct the mathematical model on which the evaluation is based are called reference data - no reference data, no model. It is, however, possible to perform an evaluation with only reference data (i.e. without any independent test data)

The Feature extraction

As soon as the reference data set contains at least one measurement it is possible to define how to extract the feature vector from the individual sensors response curves. This procedure is called feature extraction; it does not need to be started manually. Again, MultiSens software will automatically invoke the required algorithms. The main point of using feature extraction is to reduce the amount of data to be fed into the evaluation. Theoretically it would be feasible to feed the raw sensor response curves into an evaluation, with no prior treatment. However, the curves contain a very large amount of redundant information which would serve no other purpose than to blow up computation time unnecessarily. By extracting characteristic values (features) from the entire curve, a much reduced data set is obtained which (hope-fully) still retains most of the information present in the full curve. The most popular feature is the one that says by how much the sensor signal has changed during the exposition to the gaseous

sample. In MultiSens-Software parlance, this feature is called **Sig-Base**, shorthand for Signal minus Baseline. This means that the largest positive of negative deviation (Signal) from the initial value (Baseline) is extracted.

Features whose name ends in "3" use an additional averaging over three adjacent data points. Whether or not this averaging makes sense depends on the particular sensor and application.

The principal component analysis (PCA)

After feature extraction, each measurement will contribute one or several feature vectors. The feature vectors span a multi-dimensional space (feature space) where each measurement is represented by a point. The features are the base vectors for this space; if only one feature per sensor is extracted (e.g. **Sig-Base**), the feature space has as many dimensions as there are sensors.

PCA tries to find new base vectors (which are linear combinations of the original base vectors) for feature space. Thus, drawing an analogy to our familiar three-dimensional space, PCA rotates the coordinate system. Obviously, a simple rotation of the coordinate system will not help a great deal in reducing the space's dimensionality. Actually, it will not help at all.

The trick with PCA is that the new base vectors are chosen according to the variance of feature vectors. The first base vector will be chosen so that it represents the direction along which there is the largest variance; the second base vector will show the second largest variance, and so on. The base vectors thus found are then called principal components. The first principal component therefore points in the direction where the reference measurements show the greatest degree of variation.

This method will only help if the variance of feature vectors is not sufficiently well represented by the original base vectors. This is the case when there is cross sensitivity between sensors, and when the sensors are not overly selective.

The scores plot (scatter plot) shows data projected onto a plane which is spanned by two principal components. By default, the X axis is the first principal component while the Y axis corresponds to the second PC. As discussed previously, these two PCs represent the bulk of the variance present in the data set. The distance between samples corresponds directly to their degree of likeliness as "seen" by the sensors.

The scores plot is a display technology to get similarities and differences of samples at a glance.

Classification of test data

Frequently, the goal of an evaluation is the classification of an unknown sample, i.e. to determine the degree of similarity with known classes of previously analysed samples. The MultiSens software has a built-in algorithm to determine the "distance" between an unknown new sample and previously defined reference data. To this end, the program obviously needs to be told which classes the individual reference data belong to. Then, the algorithm can calculate the distance of a new sample, and select the class most frequently found in the k nearest neighbours, where k is a non-zero, user selectable integer number. This algorithm is also known as the KNN method (k-nearest-neighbours).

Additionally to the classification by the KNN method it is possible to calculate the Mahalanobis distance. The Mahalanobis distance is a value which gives the dissimilarity of a sample in respect to a certain class. A value of 0 means the sample exactly matches the class. Large values are indicating a high dissimilarity to a given class.

The computation of the Mahalanobis distance calculates the variation of samples within a class around its centre in respect to the distance of the new sample. Consequently the Mahalanobis distance takes the area of the reference data into consideration. To allow this calculation it is necessary to have enough reference data for a given class. The number of reference data points always have to be larger than the dimension of the vector space of the computation. If this doesn’t hold the program will give the output

NaN (Not a Number). Since for practical reasons the number of reference data points is low it is useful to use the scores as input data for the Mahalanobis distance. The values for the Mahalanobis distance is displayed next to the sample description. Here all distances to all classes are shown giving the description of the class first followed by the Mahalanobis distance. Additionally to the sample values the Mahalanobis distance values for the centres of the classes will be displayed next to the class description.

The principal component regression (PCR)

Principal Component Regression is an extension of the Principal Component Analysis. During calibration for each sample a certain user defined or independently measured value (e.g. a concentration value or a quality index) is assigned.

As described before the principal components are calculated. Using these principal components a multi linear regression is subsequently performed with the user defined values as target data. Resulting regression coefficients used together with the Loading values of the PCA allows the prediction of unknown samples.

The principal component analysis (PCA)

The parameters

Like the parameters for a measurement method, an evaluation's parameters are collectively displayed on several pages within one window. The first page contains settings for the feature vector, pages two and three contain lists of reference and test data, and the last page contains general parameters and classification information.

The feature vector

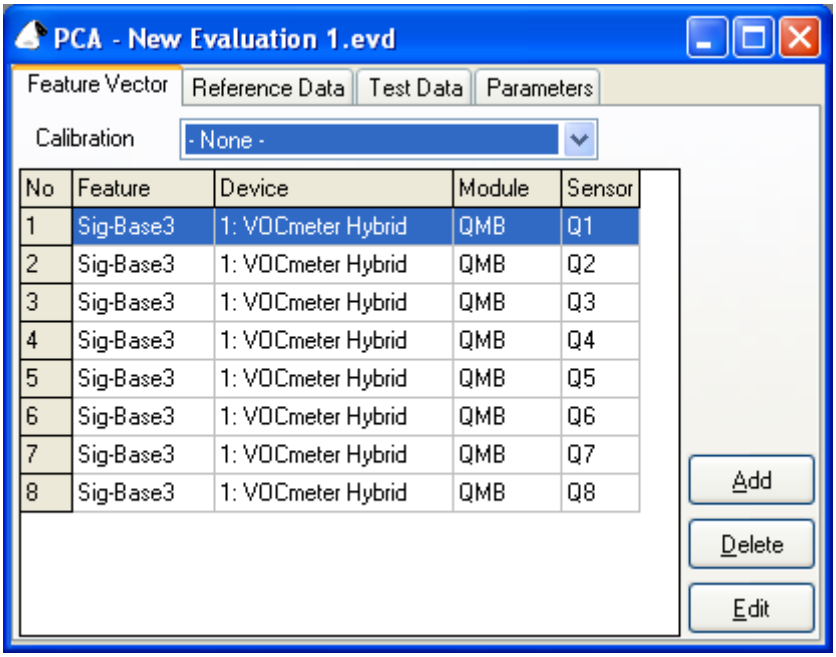
As discussed previously, the feature vector determines how to extract a small number of values from the relatively complex sensor response curves. There is a great deal of latitude in composing a feature vector. All or only some sensors may be used to build the feature vector; one sensor may be used multiple times to give its data more weight. Multiple features from one sensor can be used, too. The standard version of MultiSens software provides a choice of features. More complex features such as signal rise time and amplitude may give additional input for a subsequent evaluation and are optionally available.

The individual components of the feature vector are shown in a tabular form on this page. Each line corresponds to one feature. The sequence of features is irrelevant. Each feature is shown with a number, the type of feature, and the name of the sensor whose response curve was used to generate the feature. The sensor's name includes the module to which the sensor belongs.

New features can be introduced using the **Add** button. Once you have clicked **Add** you will first need to select a module from the list of available modules and then highlight the sensor(s) to be used in the feature extraction. Finally, select the desired type of feature extraction. The following list shows the feature extraction types currently available in the standard version of MultiSens software. Depending on the method a window requiring extra user input may show up.

Feature	Description
Sig-Base	Maximum positive or negative amplitude of the curve (signal) after the basline was subtracted. The 1st value after the start of the measurement serves as baseline value.
Sig-Base3	As Sig-Base but averaged over three values.
SigAt	Difference of the response curve at a certain point definable by the user to the baseline (at the start of the measurement).
SigAt-BaseAt	Difference of two different points of the response curve. Both points are definable by the user.

To remove a feature from the vector, highlight the respective line, and click **Delete.** The **Edit** button opens the window allowing the setting or modification of feature extraction parameters. In the case of a feature which has no user selectable parameters the Edit button has no function.



Column	Description
No	Number of the feature.
Feature	Extraction method of the feature.
Module	Module the evaluated sensor belongs to.
Sensor	Description of the sensor.

Tip: You can change the sequence of features by highlighting one feature line and then click-dragging it to a different place in the list. As mentioned before, such changes have no effect on the evaluation results.

Using the field **Calibration** allows to select the calibration method which will be applied during the evaluation, e.g. in order to reduce drift effects of the sensors.

Reference data

On the **Reference data** page you will enter those measurements that are to be included in the calculation of principal components. When you click the **Add** button, a dialog window will open which allows you to open several measurement data files simultaneously by holding down the SHIFT or CTRL key while clicking

on the files one by one, or by drawing a marquee around several files. In this window you may also change the directory clicking on it or using the symbol status line.

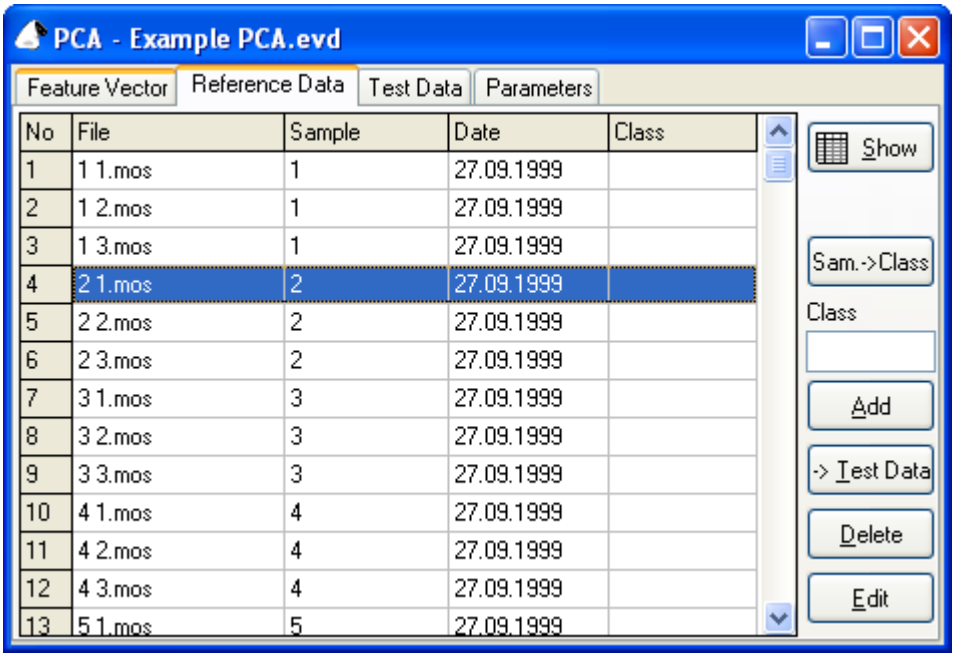
Measurements can be removed altogether by highlighting the corresponding line and clicking **Delete**, or they can be changed from reference to test data by clicking **-> Test data**

You may change the sequence of measurements as described in the previous Section. Again, the sequence is irrelevant for the results.

By clicking **Edit**, previously highlighted measurements are opened. The same result can be achieved by double clicking a measurement's file name in the table.

Using the **View** button you can look at the extracted features for the whole table as a matrix.

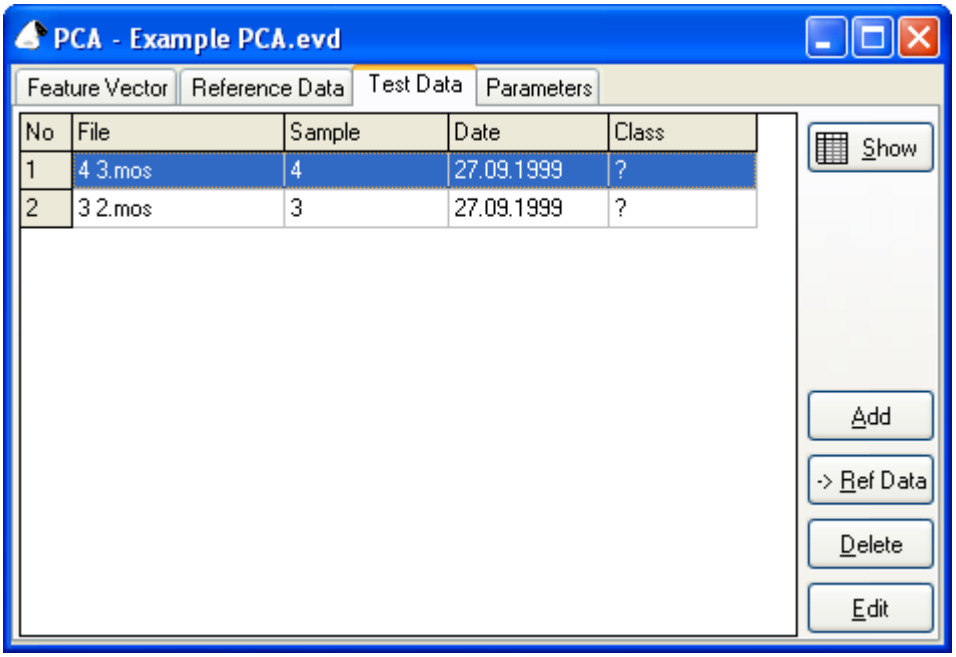
If you want to be able to have newly added test data automatically attributed to a certain class of samples, you will need to first define classes of reference data. To do this, highlight all reference measurements belonging to a certain class, and fill in a descriptive class name in the **Class** field.



Column	Description
No	Number of the measurement.
File	Filename of the measurement.
Sample	Information from the sample box of the measurement.
Class	Class the sample belongs to.

Test data

On the **Test data** page you can enter those measurements that you want to process according to the previously built model (in other words, adding more test data will not change an existing model; the principal components and the plane displayed in the scatter plot will remain the same). All buttons work in analogy to their Reference data counterparts. However, a class can not be entered. If **KNN classification** has not been selected on the **Parameter** page (see below for details), or if no classes have been defined for the reference data, a question mark will appear in the Class column. Otherwise, the class determined by the KNN algorithm will appear here.

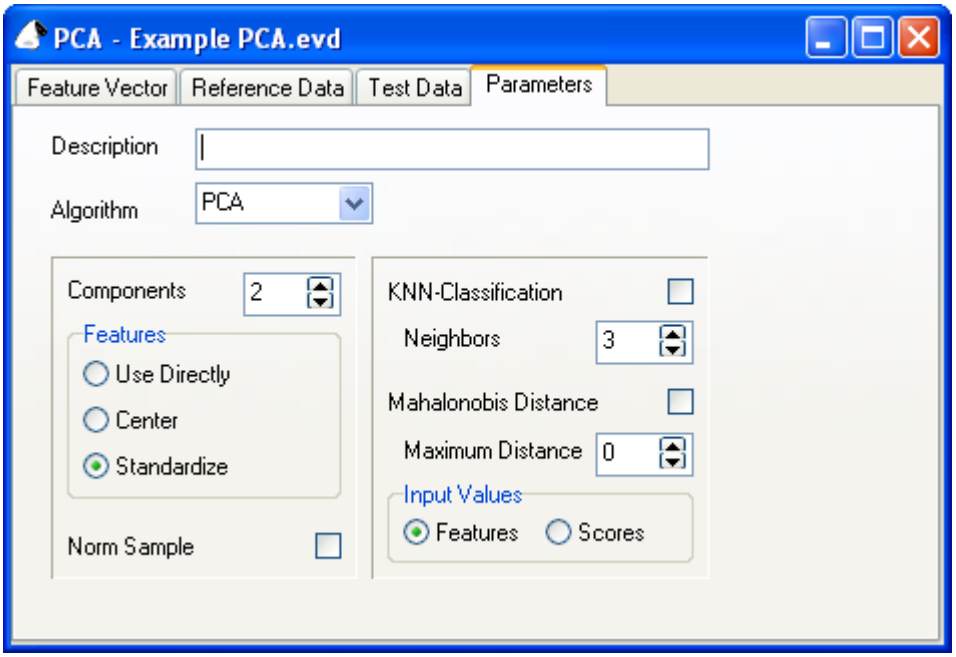


Column	Description
No	Number of the measurement.
File	Filename of the measurement.
Sample	Information from the sample box of the measurement.
Class	Class the sample belongs to.

The Parameters

On the page named **Parameter** you can set up some general parameters about the evaluation.

In the **Description** field you can enter a short descriptive text about this evaluation. The text entered here may also be made to appear in the title or subtitle of a scores or loadings plot. If the evaluation is created automatically within a task, this field is filled in from the corresponding field in the task parameters page.



Depending on which version of MultiSens you have installed, the parameter **Algorithm** lets you choose between different built in projection algorithms. The default algorithm is PCA (Principal Components Analysis).

The field **Components** defines how many principal components will be calculated. The maximum number here is the number of measurements on the Reference data page, or the number of features in the feature vector, whichever is smaller. The contents of this field has some influence on classification if scores are to be used as **Input values** (see below).

In the **Features** box , you can choose a preprocessing method for the features in the PCA. The following three options are implemented:

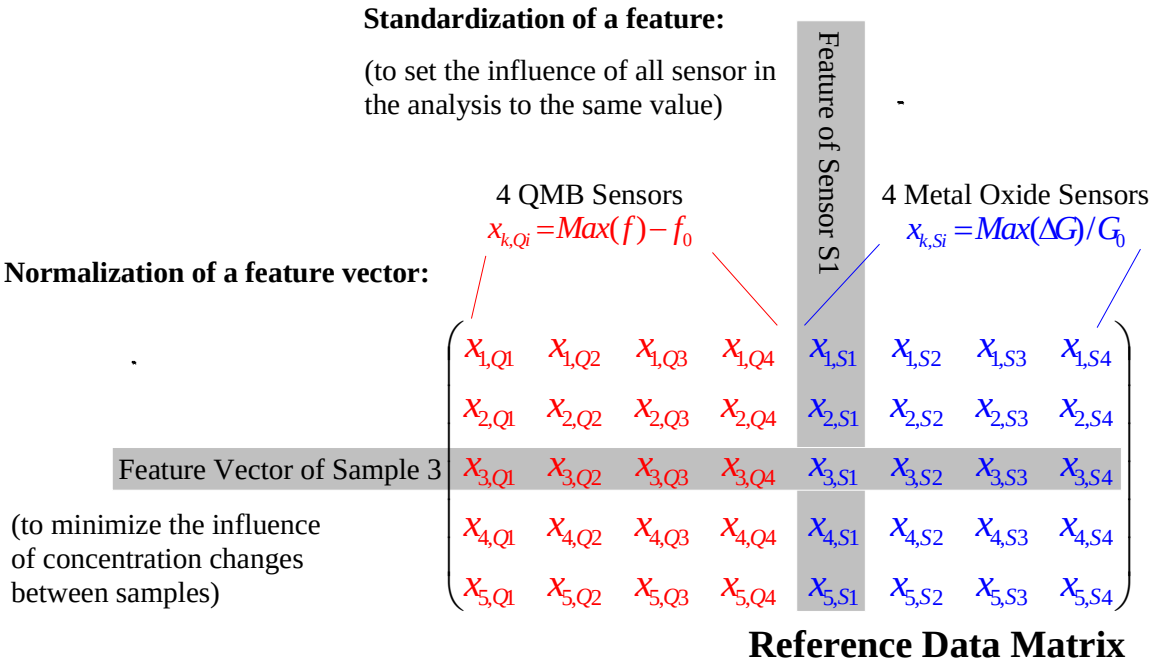
Use directly: The extracted features are not pre-processed in any way; they are used as-is.

Center: The mean value of the features in the reference data is subtracted from all features. This means that the principal components reflect only differences between features, and that the absolute feature value (which normally correlates with intensity) does not play a role. With uncentered data, the first principal component will in many cases contain mainly intensity information which is probably an unwanted property.

Standardize: With this point selected, features will be centered and additionally divided by the standard deviation of features in reference data. This means that all features will receive approximately equal weighting in the evaluation. Standardisation is recommended especially whtn different types of sensors are combined in an evaluation. Standardisation means that grossly different units (say, one sensor type in kilo-ohms, another type in milliampe'res) will cancel out, and not play a role in the evaluation.

There is a separate option **Norm samples** which can be applied in addition to any of the above. With this option activated, the length of each feature vector is forced to be one (1) without changing the relationship of features within this vector. This option is useful to minimise the influence of different intensities because normally, samples with higher concentrations will produce a longer feature vector. This simplistic explanation, however, assumes that only such features have been included whose magnitude correlates with intensity (such as Sig-Base). Additionally, this assumption is only valid for sensors showing a more or less linear response (which is not necessarily the case in real life).

The following sketch shows these relationships. We have a matrix of reference data and use x_1 , to designate the i-th feature extracted from the data of sensor j. To keep the sketch intelligible we use a simplified example with four QMB and MOS sensors each and with five samples:



Activating the combo box **Mahalanobis distance** will compute the values for all classes and samples. The vector space for this computation is the same as for the **KNN-Classification**.

If test data are to be classified automatically you will need to activate the option **KNN-CLassification**.

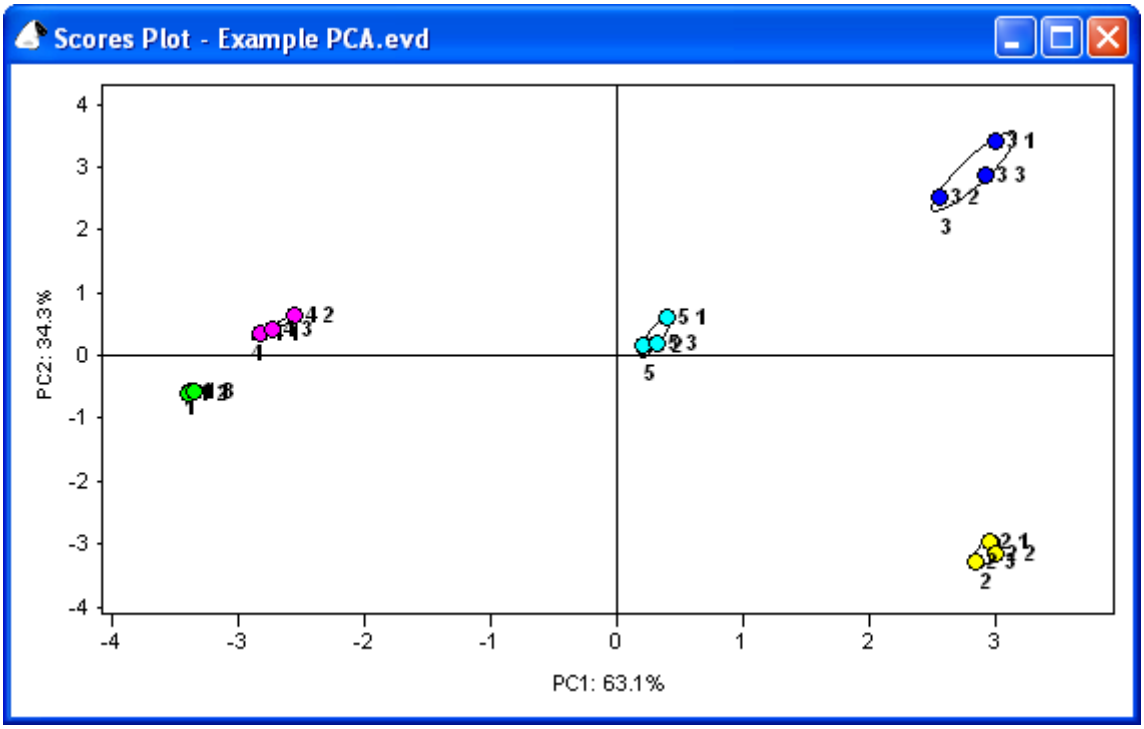
The field **Neighbors** defines how many nearest neighbours are to be used. The class appearing most frequently in the number of neighbours defined here will be chosen. If two classes appear the same number of times (which is possible only if K is an even number), the class whose sum of euclidic distances is smallest will be chosen.

The radio button field **Input values** lets you choose whether KNN and Mahalonobis distance use distances in feature space or in principal component space.

Box	Description
Description	Description of the evaluation (can be displayed as title or subtitle in the graph).
Components	Number of calculated principal components.
Features	Weighting of the features: **Use directly**: Without conversion. **Center**: Subtraction of the average from the reference data. **Standardize**: Division of the reference data by the standard deviation additionally to centering.
Norm samples	All feature vectors are recalculated to the length of one.
Mahalonobis distance	Activate the calculation of the Mahalonobis distance.
KNN-classification	Activate the automatic classification using the k-nearest-neighbor (KNN)-algorithm.
Neighbors	Number of nearest neighbors that should be considered for the classification.
Input values	Values, used for the calculation of the KNN-classification and the Mahalonobis distance: **Features**: The extracted features (after weighting and/or normalization) are used. **Scores**: The input values of the principal component analysis are used.

The scores plot

The scores plot shows a plane spanned by two principal components. The default configuration is to show the first principal component as the X axis (horizontal) and the second principal component as the Y axis (vertical). Since the first two principal components contain the largest amount of variance in the data, this diagram is a very intuitive measure of how different or similar the samples were "seen" by the sensors. The distance between points is directly proportional to the difference in features. The larger the distance between two samples in the plot the larger is the difference of the samples. The amount of variance represented by the respective principal component is shown in the axis title in the format PCx = zz.z % where X is the index of the principal component (normally 1 or 2).



The scores plot is an ideal tool for quickly grasping an overview about different samples. The score of a measurement with respect to a principal component is simply the value of the measurement on the corresponding axis. There are many options available for customizing the scores plot display.

Axes are automatically scaled so that all measurements are show in the diagram. For zooming into a certain range in the diagram, simply click-drag a rectangle around that range. By double clicking the graph or selecting **Graph - Zoom 0ff** you can revert to the unzoomed display.

By activating **Graph - Symmetric axes** it is possible to adapt scaling so that the origin of X and Y axes lies in the diagram center. If values have a strongly asymmetrical distribution around the origin, this may lead to a great deal of wasted display space.

By activating **Graph - Golden cut**, a special display mode is enforced. The ratio of X to Y axis length is forced to be the square root of two (this is the ratio used in the DIN A paper size system, and does NOT correspond to the mathematical definition of golden cut, but the initial catch phrase "golden cut" turned out to be sticky...). Additionally, X and Y axis ticks and labels are removed and replaced by only the ratio of the ranges displayed on the X and Y axes (PC x : PC y = z.zzz). This display mode may be useful for comparing the results of different evaluations with one another.

By activating **Graph - Equal scale**, scalings are adjusted so that unit lengths along X and Y axes are identical, i.e. 1cm along the X axis corresponds to the same number of units as 1 cm along the Y axis.

The Symmetric axes, Golden cut, and Equal Scale settings may also be combined arbitrarily.

The menu points **Graph - X-axis** and **Graph - Y-axis**, respectively, allow you to define which principal component will be shown along which axis. This way it is also possible to use different combinations than the default (PC 1: X PC 2: Y). You may, for example, choose to display PC 3 vs PC 2.

If you have defined classes for your reference data, classes can be emphasized in the plot by ellipses drawn around samples belonging to the same class **Graph - Ellipsis**. There are several options here. First, ellipses can be calculated so that their principal axes correspond to three times the standard deviation of scores with respect to the corresponding principal component, independently for X and Y axes **Graph – Ellipsis Independent**. Alternatively, ellipses can be calculated so that the correlation between the principal components within the class is taken into account **Graph – Ellipsis Correlated**. In this case, the principal axes correspond directly to standard deviation (not three times as in the previous case). N.B.: These two options are not mutually exclusive! If you activate both of them you will get two different ellipses for each class. It is also possible to have the class name displayed next to the ellipse **Graph – Ellipsis Caption**, and to display the ellipse axes **Graph – Ellipsis Draw axes**.

Individual measurements can be displayed in different ways. Classes of reference data can be distinguished by different colours (**Graph - Symbols – Mark classes by color**) or by different shape (**Graph - Symbols – Mark classes by shape**). This is applicable for Test data as well. (**Graph - Symbols – Mark Test data by color**, **Graph – Symbols – Mark Test data by size**). Reference data are represented by circles, Test data are represented by diamonds.

Labels may be chosen (**Graph - Label**) from the number of the measurement in the table of reference or test data (**Graph - Label - Number**), the filename of the corresponding measurement (**Graph - Label - Filename**), the description of the sample (**Graph - Label - Sample**) and the name of the class to which the measurement belongs (**Graph - Label - Class**).

For easier filing and finding diagrams, top and bottom titles may be added to a plot below and/or above the diagram (**Graph - Title – Title above…**) and/or (**Graph - Title – Title below…**). Once either of these two menu points has been selected, a dialog window will pop up which will prompt you for the title text, its alignment (left, right, centered), and, optionally, font and size. If you have made your choice you have an option to make it permanent by clicking **As Standard** which will make these settings appear automatically as the default setting in the future. By clicking **Standard**, the current default settings are applied to the current title. It is possible to use macros in the tide text, creating variable content that is updated automatically from data entered elsewhere in the evaluation. The following table gives details:

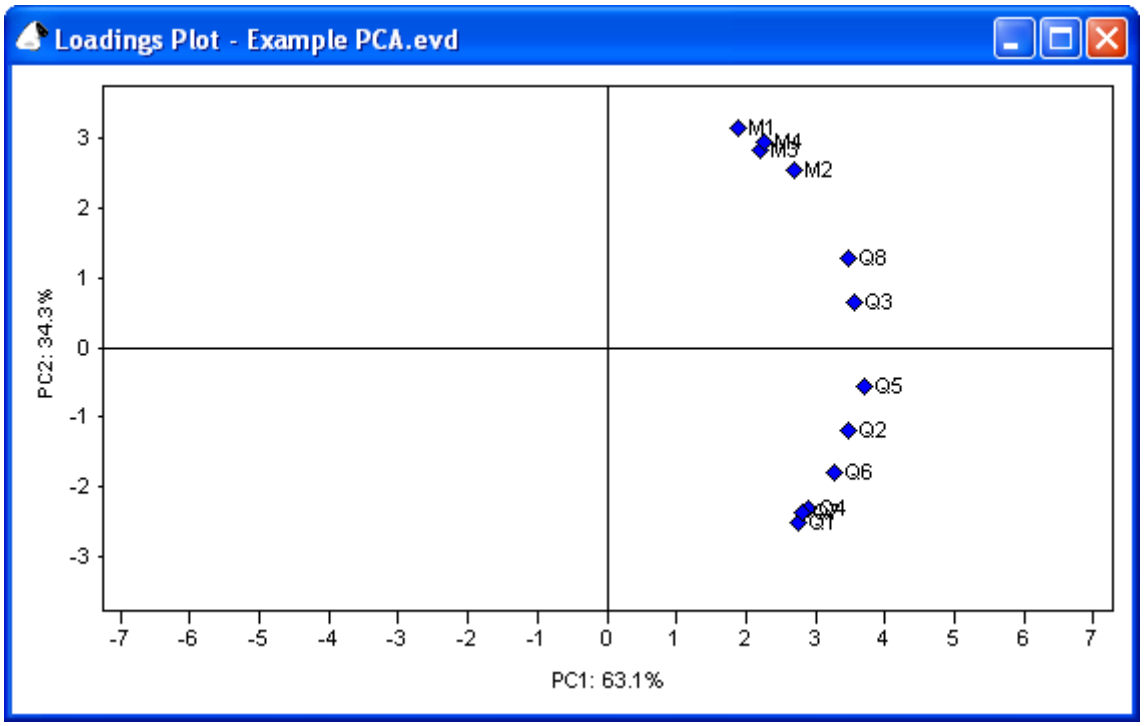
Macro	Function	Description
{Description}	Description	Shows the information of the description box.
{Filename}	Filename	Shows the filename and the path.
{Now}	Now	Shows the current time.
{ProgramVersion}	Software version	Shows the name and the version of the program.
{Today}	Today	Shows the current date.
{User}	User	Shows the name of the user (the login under Windows).

*Tip: A graph can be transferred to the clipboard by **Edit – Copy**. This allows to „copy and paste" graphs into different applications (e.g. Word-processors)*

The loadings plot

The loadings plot shows to which extent individual features contribute to the calculation of principal components. The further "inside" (close to the origin) a feature lies, the smaller its influence. The more distant from the origin, the more important. The azimuthal distribution of features gives hints about the

data set's redundancy. Features providing very similar information are found very close to each other azimuthally (under the same angle). Features providing vastly different information will be located under clearly separated angles.



The same axis scaling options as for the scores plot (**Graph - Symmetric axes**, **Graph - Equal scale**, **Graph - Zoom off**)are applicable here.

Additionally, loadings can be weighted with their corresponding eigenvalues (**Graph - Weight with Eigenvalues**).

Again, options are available for selecting which principal component to display on which axis (**Graph - X-axis** and **Graph - Y-axis**).

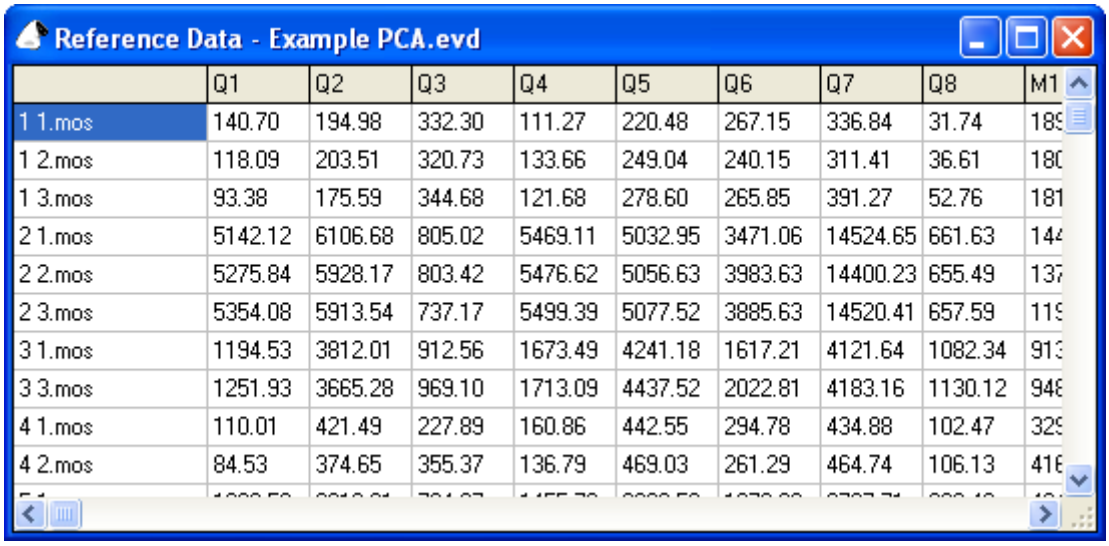
Again, there is the possibility of using symbols and/or captions for the features. If symbols are chosen (**Graph - Symbols activated**), all features are shown as diamonds.

Labeloptions available are the number of the feature within the feature vector (**Graph – Label - Number**) , the name of the sensor used for the extraction of this feature (**Graph – Label - Sensor**), and a comprehensive caption including module, sensor, and feature extraction method names (**Graph – Label - Sensor+Method**).

Title options are identical to those available with the scores plot. The same macros are applicable.

Output of numerical values

While it is very convenient and intuitive to view the results graphically, sometimes it may be useful to have access to processing results in tabular or matrix form. MultiSens software offers that possibility too.



	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	M1
1 1.mos	140.70	194.98	332.30	111.27	220.48	267.15	336.84	31.74	189
1 2.mos	118.09	203.51	320.73	133.66	249.04	240.15	311.41	36.61	180
1 3.mos	93.38	175.59	344.68	121.68	278.60	265.85	391.27	52.76	181
2 1.mos	5142.12	6106.68	805.02	5469.11	5032.95	3471.06	14524.65	661.63	144
2 2.mos	5275.84	5928.17	803.42	5476.62	5056.63	3983.63	14400.23	655.49	137
2 3.mos	5354.08	5913.54	737.17	5499.39	5077.52	3885.63	14520.41	657.59	119
3 1.mos	1194.53	3812.01	912.56	1673.49	4241.18	1617.21	4121.64	1082.34	913
3 3.mos	1251.93	3665.28	969.10	1713.09	4437.52	2022.81	4183.16	1130.12	948
4 1.mos	110.01	421.49	227.89	160.86	442.55	294.78	434.88	102.47	329
4 2.mos	84.53	374.65	355.37	136.79	469.03	261.29	464.74	106.13	416

The menu **Evaluation – Matrix** accesses the following menu points

Features	Shows values of the features extracted from the reference measurements (**Reference data**) or the test data (**Test data**).
Scores	Shows the calculated scores of the principal components of the **Reference data** or **Test data**.
Loadings	Shows the loadings of all features.
Variances	Shows the information content as percentage for each principal component.
Mahalonobis distance	Shows the Mahalonobis distance between the **Classes**, or between the **Reference data** and the classes, or between the **Test data** and the classes.

Once a matrix is displayed, the menu point **Matrix - Transpose** lets you swap rows and columns.

For the reference data, test data, and scores matrices, **Matrix - Sample description** lets you choose between the number of this feature (**Number**), the measurement's file name (**File name**), the contents of the samp1e field in the measurement (**Samp1e**), or the class attributed to this measurement (**class**).

For the reference data, test data, and loadings matrices, feature labels can be chosen with **Matrix - Feature Label** from the following choices: the number of the feature in the feature vector (**Number**), the name of the sensor used for the extraction of this feature (**Sensor**), and a comprehensive label including module, sensor, and feature extraction method names (**Sensor+Method**).

For the matrix of loadings, you can additionally enable weighting with eigenvalues (**Matrix - Weight with eigenvalues**).

Export of results

For exporting results to other applications, you can generally use the familiar mechanism of **Edit - Copy** and **Edit - Paste**. For exporting PCA results (scores and loadings), more elaborate possibilities exist. You can choose to copy the entire matrix including all values and all labels (**Edit - Copy all**), or you first highlight the values you wish to copy. Then you have a choice of either copying just the numeric values with **Edit - Copy**, or you use **Edit - Copy with label** to include label information.

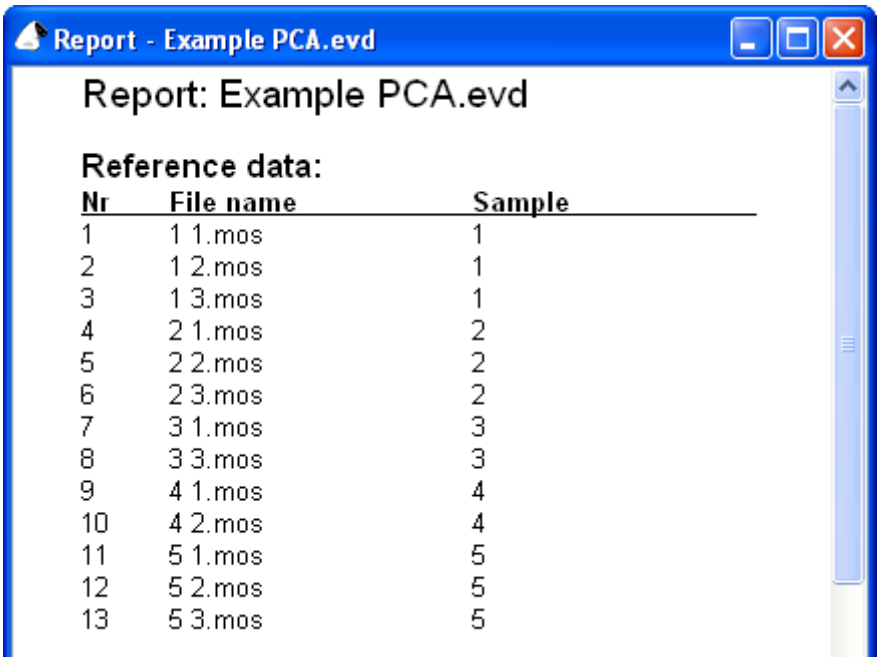
The clipboard contains all data as text, the delimiter is the tab-symbol. The decimal delimiter is a dot. This is independent of settings in the control panel of Windows™.

Hint: Before pasting data from the clipboard to a application program it might be necessary to adapt the settings in the control panel. The decimal delimiter must be set to a dot. After adjustment you might have to re-start the application program in which you want to paste the data.

The report

The report allows to document the results of an evaluation in text form. The MultiSens-software allows to create a report of a evaluation by the menu **Evaluation – Report**. This command opens a window which shows the report. The standard version of MultiSens contains two report template: Standard.rtf and Extended.rtf. A box in the icon bar allows to switch between the two versions.

The report is dynamically linked to the evaluation. It is not possible to change the report in the MultiSens software. The template can be transferred into an external word processor by Copy and Paste and can be modified. **File - Print** prints the report.



Nr	File name	Sample
1	1 1.mos	1
2	1 2.mos	1
3	1 3.mos	1
4	2 1.mos	2
5	2 2.mos	2
6	2 3.mos	2
7	3 1.mos	3
8	3 3.mos	3
9	4 1.mos	4
10	4 2.mos	4
11	5 1.mos	5
12	5 2.mos	5
13	5 3.mos	5

The principal component regression (PCR)

Principal component regression (PCR) will be available to you, if you acquired MultiSens including the option ‘PCR’.

Principal component regression is a regression algorithm for quantification. Rather then assigning measured samples to different classes, a value will be assigned.

Like in the principal component analysis, in the first step the principal components (scores) are calculated; thus scores plot and loadings plot can be plotted.

The user has to fill in a value for every sample of the reference data set. Applying multilinear regression a model is built to allow the calculation of that user defined value from the scores.

To check the quality of the model, the prediction values are also calculated for the reference data. On the true / predicted plot the true values (as defined by the user) are plotted against the predicted values (by the model). This graph visualizes the prediction accuracy of the model. As there are no true values for the test data, only reference data are shown on this graph.

In the results plot the predicted values of all samples (within the reference and test data) are shown as bar graph.

The prediction accuracy of the model within the reference data will increase the more components (scores) are used in the calculation. The prediction accuracy within the test data however, will decrease in general if the number of components is increased beyond a certain number. This paradoxical behavior results from the fact that in the creation of the model the true values of the reference data are known. The more components in the regression are used, the higher the freedom of the model will be to adopt to these known values. As also the reference data will have a certain amount of measurement error, the influence of this error increases (in most cases) with the number of components. If such an overfitted model is used to predict test data the random measurement error of the reference data may lead to totally wrong results. While setting up an evaluation using PCR one should always check the model by inserting samples not included in the reference data set into the test data set where true values are known. The error in the prediction these test data should then be checked critically and compared to the error on reference data (validation).

The parameters

As for the PCA, an PCR's parameters are collectively displayed on several pages within one window. The first page contains settings for the feature vector, pages two and three contain lists of reference and test data, and the last page contains general and regression parameters.

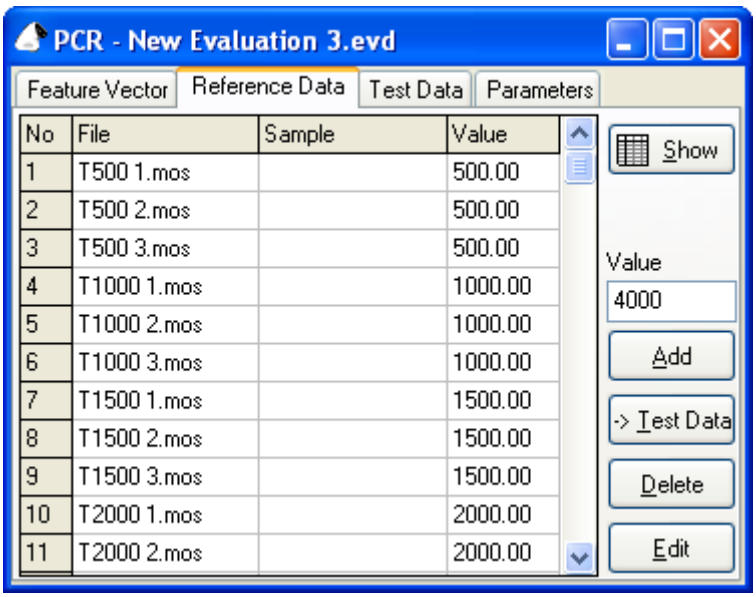
The feature vector

The functionality of the feature vector is identical to that one of the PCA described in chapter 0.

Reference data

As described in 0 on the page reference data the reference data set is composed.

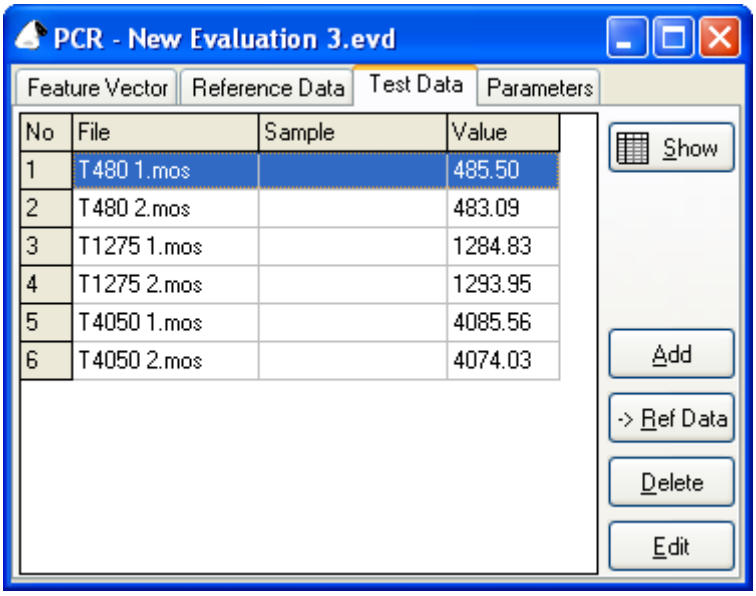
Instead of a class a value is assigned to each individual member of the reference data set. The following table explains the different columns on this page.



Column	Description
No	Number of the measurement.
File	Filename of the measurement.
Sample	Information from the sample box of the measurement.
Value	(true) value that should be related to the measurement.

Test data

On the page test data the measurements are defined, that you want to evaluate on the bases of the model calculated from the reference data set. As the values of the test data are calculated automatically, it is not possible to input any data in the column Value.



Column	Description
No	Number of the measurement.
File	Filename of the measurement.
Sample	Information from the sample box of the measurement.
Value	(predicted) value, calculated for this measurement.

The parameters

On the page named **Parameter** you can set up some general parameters about the evaluation.

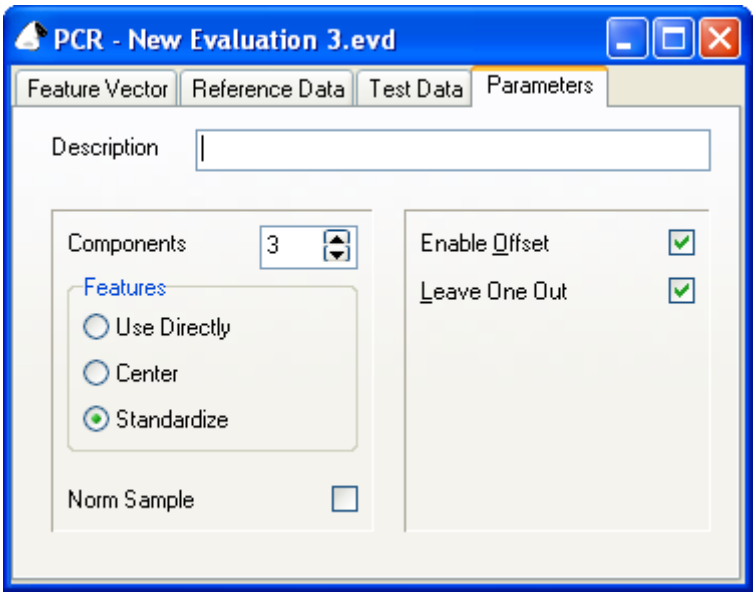
In the **Description** field you can enter a short descriptive text about this evaluation. The text entered here may also be made to appear in the title or subtitle of a scores or loadings plot. If the evaluation is created automatically within a task, this field is filled in from the corresponding field in the task parameters page.

The field **Components** defines how many principal components will be calculated. The maximum number here is the number of measurements on the Reference data page, or the number of features in the feature vector, whichever is smaller.

The contents of this field will also define, how many input values are used for the regression. As discussed in 0 the choice of number of components used in the PCR is a critical parameter that should be chosen with grate care.

In the **Features** box , you can choose a preprocessing method for the features in the PCR. This parameter and the parameter **Norm samples** has been discussed in great detail in chapter 0.

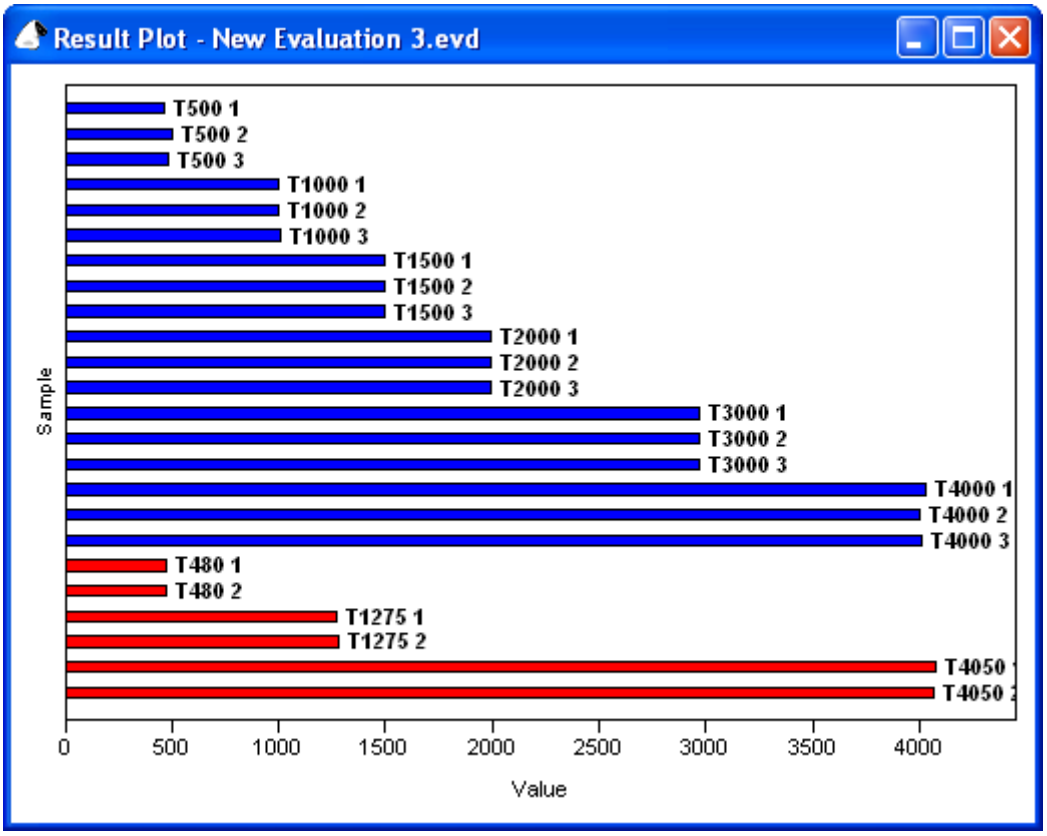
The Option Enable offset relates to the calculation of the multilinear regression of the scores onto the result values and in practice should be enabled always. In some rare cases (e.g. when the features are used directly without centering or standardization and a proportional relation without any offset is assumed between the features and the target values) it might be appropriate to disable this option.



Box	Description
Description	Description of the evaluation (can be displayed as title or subtitle in the graph).
Components	Number of principal components calculated and considered for the regression.
Features	Weighting of the features: **Use directly**: Without conversion. **Center**: Subtraction of the average from the reference data. **Standardize**: Division of the reference data by the standard deviation additionally to centering.
Norm samples	All feature vectors are recalculated to the length of one.
Offset enable	Offset enabled for the calculation of the regression coefficient.

The bar chart

The result plot visualizes the results of the PCR as horizontal bar chart. The single measurements are represented as bars. Positive values wil be shown as bars extending to the right, negative values will extend to the left. Using the menu option **Graph –Zero** the origin can be included in the horizontal range.Using **Graph - Draw** bars can be removed totally (**Only text**) or can be displayed as **Bars** or **Points**. With **Graph – Label** the text that is displayed for each sample can be chosen (**None**, **Number**, **File name**, **Sample**, **Value**). With **Graph – Title** the titles above (**Title above**) and below (**Title below)** van be defined. Like in any graph macros can be used within the title text (see chapter 0).



The true/predicted plot

In order to visualize the prediction accuracy of the model, on this graph the predicted values (calculated by the model) are plotted against the true values (as defined by the user).

Each sample of the reference data is represented by a point, whose coordinates on the X-axis are true values and on the Y-Axis are the predicted values. If all samples are represented on a straight line that links zero and the point (1/1) then the reference data is predicted with no error. As mentioned in 0 for judging the quality of the model one has to check also the error made in the prediction of known test data, that is not included in the reference data set (validation).

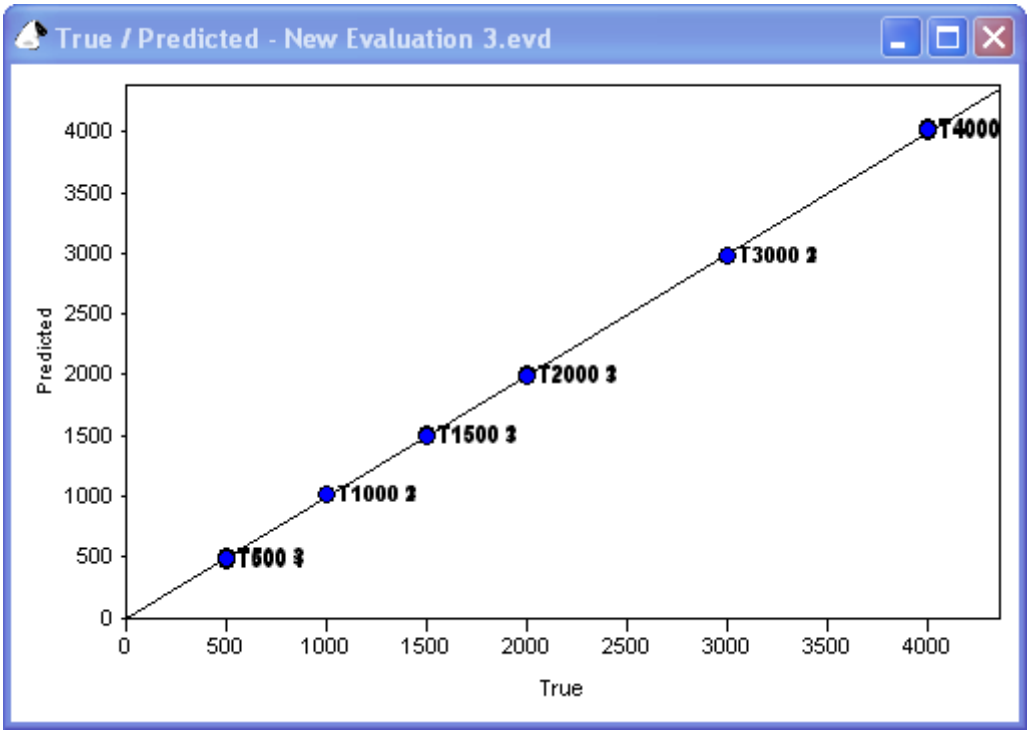
By default the axes will be scaled, so that the origin of the axes will be on the graph. If **Graph – Zero** is deactivated the axes will be scaled in order to show all samples in the diagram without wasting any space.

By activating **Graph - Symmetric axes** it is possible to adapt scaling so that the origin of X and Y axes lies in the diagram center. By activating **Graph - Equal scale**, scalings are adjusted so that unit lengths along X and Y axes are identical, i.e. 1cm along the X axis corresponds to the same number of units as 1 cm along the Y axis. The line respresenting correctly predicted reference data will then have an angle of 45 degree.

The settings ‚**Zero'**, , **Symmetric axes**' and , **Equal scale**' can be combined.

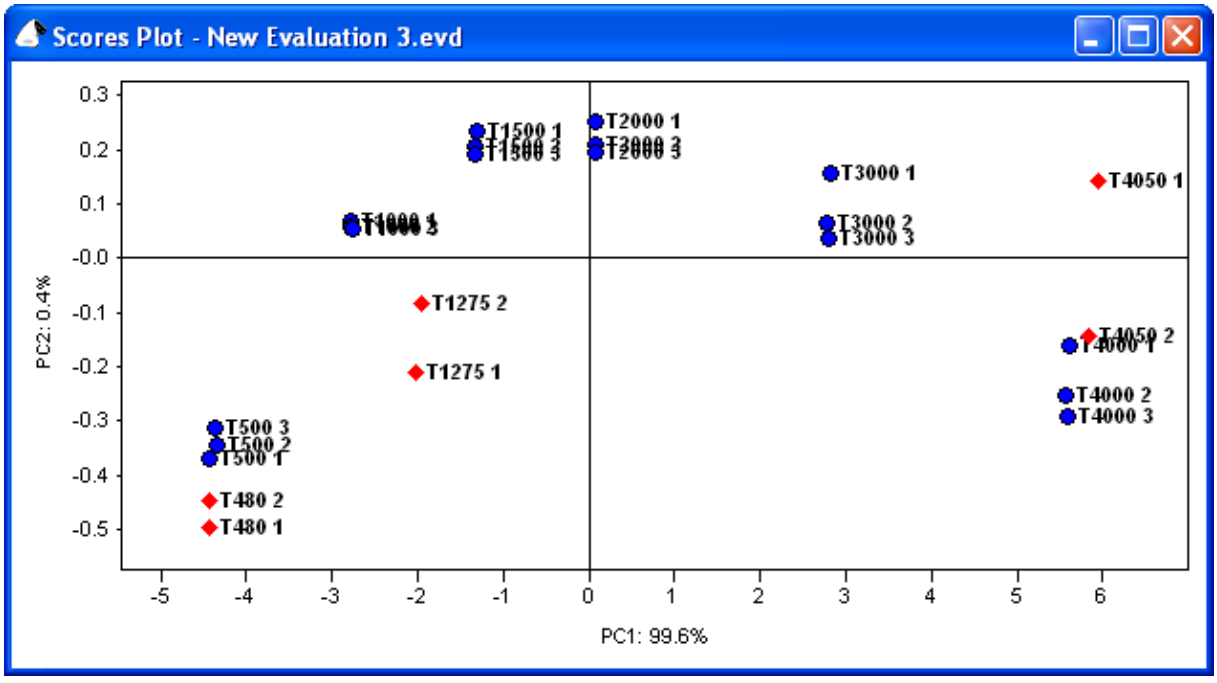
Labels may be chosen (**Graph - Label**) from the number of the measurement in the table of reference data (**Graph - Label - Number**), the filename of the corresponding measurement (**Graph - Label - Filename**), the description of the sample (**Graph – Label - Sample**) and the true value assigned by the user (**Graph - Label - Value**).

For documentation purposes titles can be assigned like in any other graph (**Graph - Title**).



The scores plot

The scores plot shows a plane spanned by two principal components. The default configuration is to show the first principal component as the X axis (horizontal) and the second principal component as the Y axis (vertical). Since the first two principal components contain the largest amount of variance in the data, this diagram is a very intuitive measure of how different or similar the samples were "seen" by the sensors. The distance between points is directly proportional to the difference in features. The larger the distance between two samples in the plot the larger is the difference of the samples. The amount of variance represented by the respective principal component is shown in the axis title in the format PCx = zz.z % where X is the index of the principal component (normally 1 or 2).



The scores plot is an ideal tool for quickly grasping an overview about different samples. The score of a measurement with respect to a principal component is simply the value of the measurement on the corresponding axis. There are many options available for customizing the scores plot display.

Axes are automatically scaled so that all measurements are show in the diagram. For zooming into a certain range in the diagram, simply click-drag a rectangle around that range. By double clicking the graph or selecting **Graph - Zoom off** you can revert to the unzoomed display.

By activating **Graph - Symmetric axes** it is possible to adapt scaling so that the origin of X and Y axes lies in the diagram center. If values have a strongly asymmetrical distribution around the origin, this may lead to a great deal of wasted display space.

By activating **Graph - Golden cut**, a special display mode is enforced. The ratio of X to Y axis length is forced to be the square root of two (this is the ratio used in the DIN A paper size system, and does NOT correspond to the mathematical definition of golden cut, but the initial catch phrase "golden cut" turned out to be sticky...). Additionally, X and Y axis ticks and labels are removed and replaced by only the ratio of the ranges displayed on the X and Y axes (PC x : PC y = z.zzz). This display mode may be useful for comparing the results of different evaluations with one another.

By activating **Graph - Equal scale**, scalings are adjusted so that unit lengths along X and Y axes are identical, i.e. 1cm along the X axis corresponds to the same number of units as 1 cm along the Y axis.

The Symmetric axes, Golden cut, and Equal Scale settings may also be combined arbitrarily.

The menu points **Graph - X-axis** and **Graph - Y-axis**, respectively, allow you to define which principal component will be shown along which axis. This way it is also possible to use different combinations than the default (PC 1: X PC 2: Y). You may, for example, choose to display PC 3 vs PC 2.

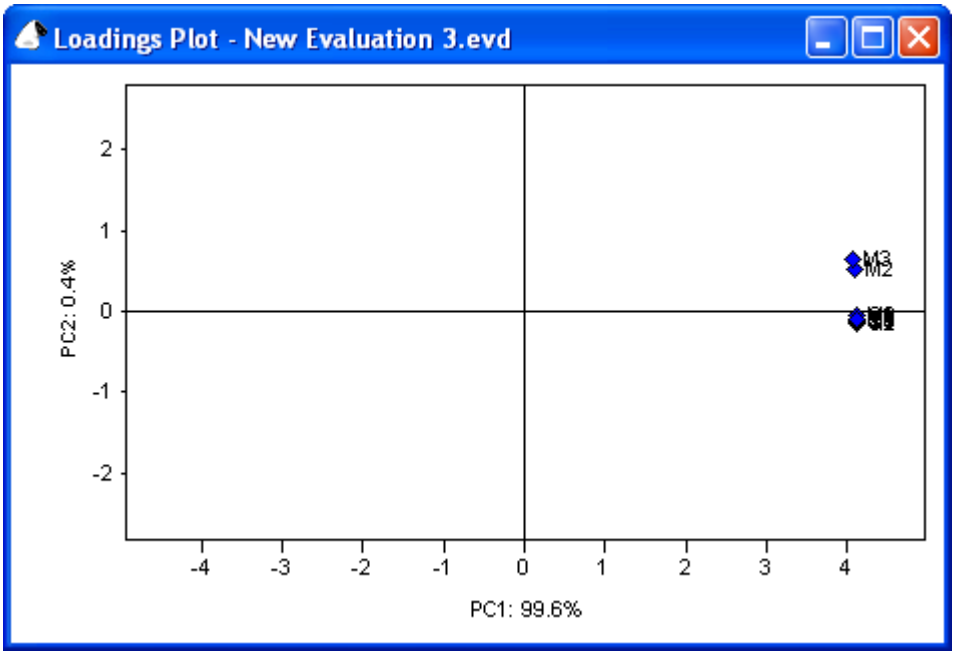
If **Graph - Symbols** is activated reference data are represented by blue circles, and test data are represented by red diamonds.

Labels may be chosen (**Graph - Label**) from the number of the measurement in the table of reference or test data (**Graph - Label - Number**), the filename of the corresponding measurement (**Graph - Label - Filename**), the description of the sample (**Graph - Label - Sample**) and the value assigned by the user in the case of reference data or calculated by the model in the case of test data (**Graph - Label - Value**).

In **Graph – Title** corredsponding titles for the graph can be assigned.

The loadings plot

The loadings plot shows to which extent individual features contribute to the calculation of principal components. The further "inside" (close to the origin) a feature lies, the smaller its influence. The more distant from the origin, the more important. The azimuthal distribution of features gives hints about the data set's redundancy. Features providing very similar information are found very close to each other azimuthally (under the same angle). Features providing vastly different information will be located under clearly separated angles.



The same axis scaling options as for the scores plot (**Graph - Symmetric axes**, **Graph - Equal scale**, **Graph - Zoom off**)are applicable here.

Additionally, loadings can be weighted with their corresponding eigenvalues (**Graph - Weight with Eigenvalues**).

Options are available for selecting which principal component to display on which axis (**Graph - X-axis** and **Graph - Y-axis**).

Again, there is the possibility of using symbols and/or captions for the features. If symbols are chosen (**Graph - Symbols** activated), all features are shown as diamonds.

Labels options available are the number of the feature within the feature vector (**Graph – Label - Number**) , the name of the sensor used for the extraction of this feature (**Graph – Label - Sensor**), and a comprehensive caption including module, sensor, and feature extraction method names (**Graph – Label - Sensor+Method**).

Title options are identical to those available with the scores plot. The same macros are applicable.

Output of numerical values

The menu **Evaluation – Matrix** accesses the following menu points

Features	Shows values of the features extracted from the reference measurements (**Reference data**) or the test data (**Test data**).
Scores	Shows the calculated scores of the principal components of the **Reference data** or **Test data**.
Loadings	Shows the loadings of all features.
Result values	Shows the true and predicted values of the **Reference data** or the predicted values of the **Test data**.

The report

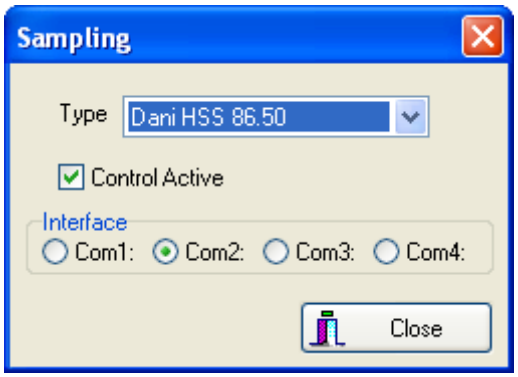
The report window of the PCR is practically identical to that one of the PCA and has already been described in chapter 0. Differences result merely from applicable macros (see appendix).

Options

Sampling

The corresponding menu point is Options - Sampling. Here, you simply have a choice of **None**, **Dani HSS 86.50** or **HP 7694**. Please choose the correct type of sampling attached to your device.

The Dani HSS 86.50 can be controlled via a serial port. If you want to control this Headspacesampler with MultiSens activate the option **Control active** and the serial port the Dani is connected to.

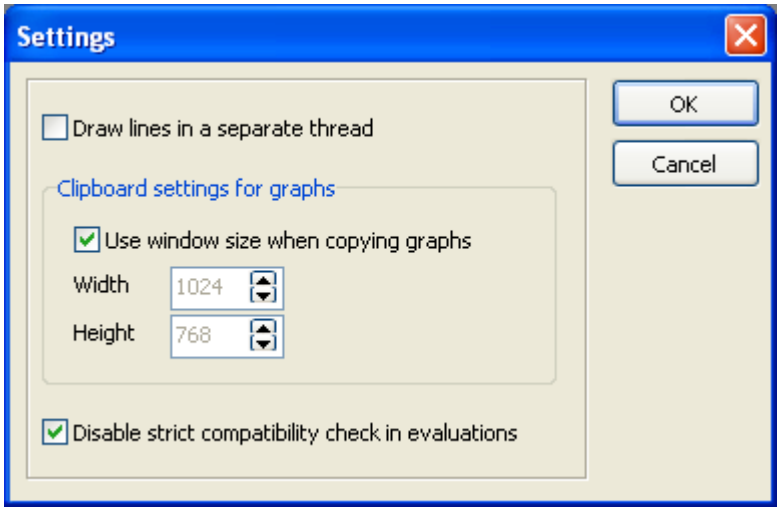


Set-up of Devices

In the menu choose **Options – Set-up of Devices**. A dialog will be shown, where you can add devices to the set-up of MultiSens. Depending on the type of device an **Interface** and/or **Configuration** dialog is available. Further details can be found in *chapter 1.3 Configuration of the Devices*.

Settings

The Settings dialog allows to set various properties of the MultiSens program.



If **Draw lines in a separate thread** is activated, the graph display of measurement data will use separate thread to draw the sensor responses. On slow computers, measurement data may by acquired faster than the computer can draw the corresponding graphs (especially when many sensors and long measurements are acquired at a fast interval rate). As a result the program may not be able to react to user input. This can be prevented, when this setting is enabled.

Clipboard settings for graphs determine how graphs are exported to the clipboard (using **Edit – Copy**). For publications and reports it is often desired, to have consistent scaling of graphics. In that case disable **Use window size when copying graphs** and set **Width** and **Height** to desired values. The graphs are

exported as vector graphics (windows meta file), however the resolution and size of fonts depends on these settings.

Disable strict compatibility check in evaluations influences, how MultiSens will examine measurements that are combined into one evaluation. Whenever you add a new measurement to an evaluation, a check is performed to make sure, that the same set-up is used in both measurements. Measurements with different set-ups (e.g. different number or types of devices) can not be combined in one evaluation and will be rejected. If the set-ups are matching another check is performed to compare the parameters used in the measurements. If differences in the parameters are found, a warning message is presented and the user may decide whether to include the measurement or not. If this option is enabled this additional check will not be performed and no warning will be given when combining measurements with diverging parameter sets.

Work directory

The menu entry **Options – Work directory** brings up a dialog where the directory is selected that you normally will store your files to. If you save or open files in MultiSens this work directory will be the default in the file save / file open dialogs.

Start MATLAB Server / Start Excel Server

MultiSens is using MATLAB and Excel for data export. These options will be checked when MultiSens has started the respective program in the background. Clicking on the Option will manually load or unload the external program.

Both MATLAB and Excel may be loaded without being visible on the computer. This is the default way, MultiSens will load the programs, unless Excel or MATLAB has not already been running visibly.

Setting of the symbol and status bar

With **Options – Icon bar** and **Options – Status bar** the display of the corresponding bar can be enabled or disabled. On small display (e.g. Notebooks) you can save some space on your desktop using these options. Some settings might not be accessible without activated icon bar!.

Appendix

Macros

Macros are used in the title box within the MultiSens software. Using a macro text information of a measurement or an evaluation can be generated. A macro is always incorporated in curly brackets. In the following table available macros are listed:

Macro	Function	Description
{Description}	Description	Shows the information of the description box.
{Filename}	Filename	Shows the filename and the path of the evaluation.
{Now}	Now	Shows the current time.
{Program}	Name of the programme	Shows the name of the programme.
{ProgramVersion}	Software version	Shows the name and the version of the programme.
{Today}	Today	Shows the current date.
{User}	User	Shows the name of the user (the login under Windows).
{Version}	Version	Shows the version of the software.

The following macros are defined for the representation of measurements:

Macro	Function	Description
{Date}	Date	Shows the date of the measurement.
{Time}	Time	Shows the time of the measurement.

The following macros are defined for the representation of evaluations:

Macro	Function	Description
{Type}	Type	Shows the type of evaluation (PCA or PCR).
{Calibration}	Calibration	Shows the filename of the calibration method (without the path).