PhotoKat Software

User Manual
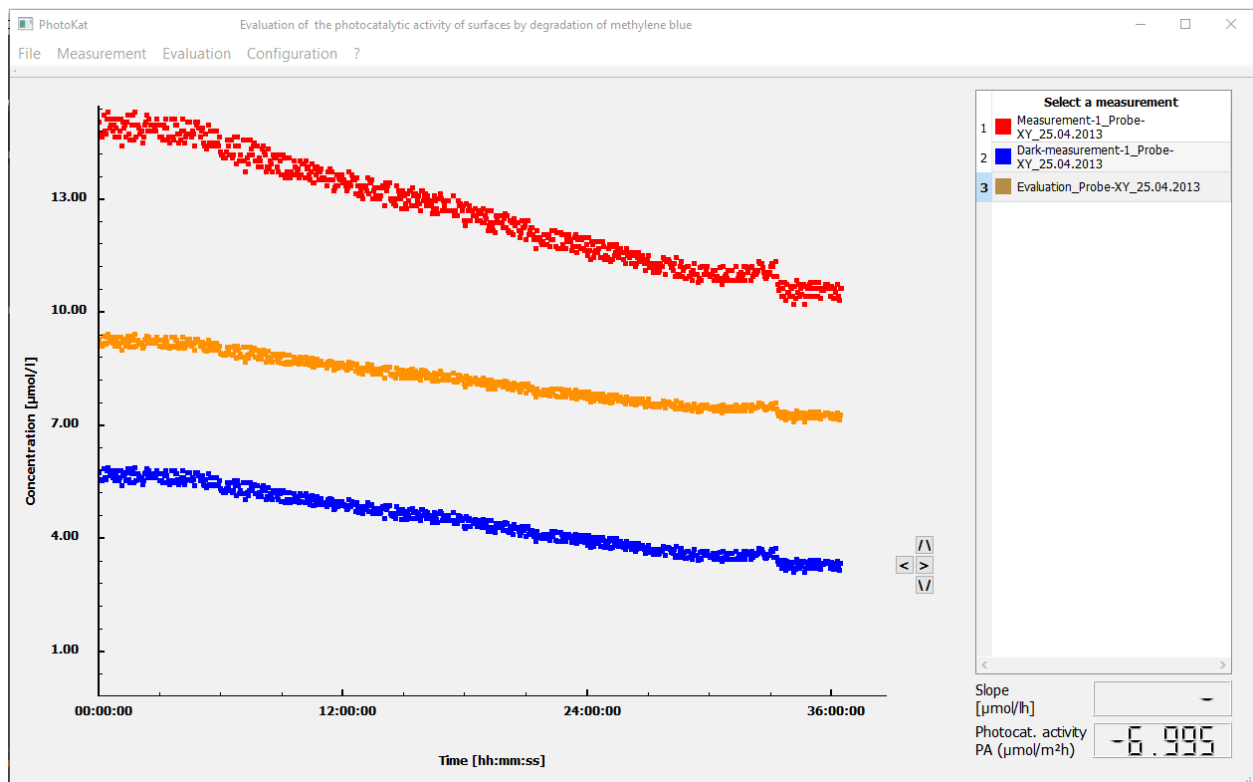
Content

1. General description

The *PhotoKat* evaluation software enables the recording, graphical visualisation, and evaluation of data in investigations of the photocatalytic activity of surfaces by measuring the degradation of methylene blue. The evaluation of the measured data is based on the German standard DIN 52980 in its version of October 2008 and the international standard ISO 10678 in its version of September 2010. The software is intended to be used in combination with the transmission measurement system of MRC Systems GmbH.

The absorbance data of the methylene blue solution are measured by the transmission measurement system, recorded by a data logger, and transferred to the evaluation software via USB. The recorded data enable the quantitative evaluation of the photocatalytic activity of material samples by means of calculating the degradation rate of methylene blue.

2. System requirements

The *PhotoKat* evaluation software can be used with common Windows computers. The measurement requires a data logger which must be connected before the start of the measurement.

3. Installation and start of the program

1) To install the *PhotoKat* evaluation software copy all files from the directory Photokat-[version number] of the delivered CD-ROM into an arbitrary directory of your computer.

2) Connect the data logger to a USB port of your computer.

3) Install the RedLab software, which you find on the delivered RedLab CD.

4) Call the RedLab software "InstaCal" once. The data logger will be recognized by the software and can be used from now on. Click on "board configuration" and select the option "8 Single Ended" in "No. of Channels".

5) To start the program open the file "PhotoKat.exe", which you find in the subdirectory /bin of the program directory.

Note:
As long as "InstaCal" was not initialised as described in step 4, you will see an error message "Invalid board number" whenever you try to start the measurement.

4. Program window

The user interface of the software is divided into the following four sections:

a) Menu bar
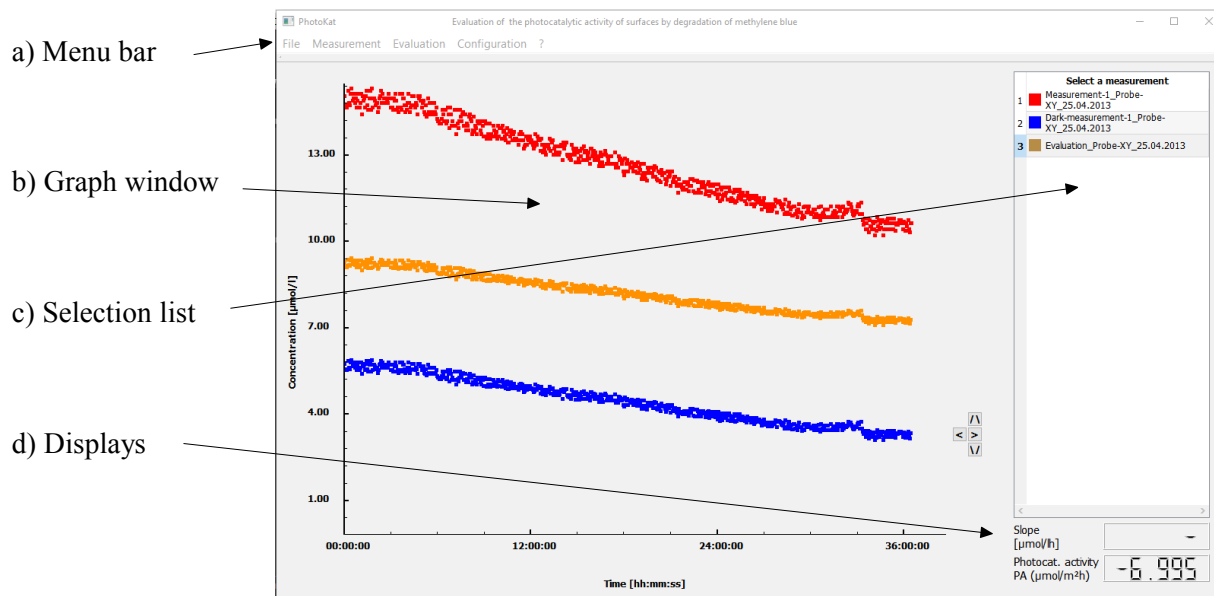
b) Graph window

c) Selection list

d) Displays

Figure 1: User interface of the PhotoKat evaluation software. In this example the program window is shown during an evaluation (see below). During a measurement the window looks similar. Instead of concentrations the voltages and on the right bottom further measured values are displayed.

5. Quick guide

5.1. Measurement

- Before you start a measurement make sure that the USB connection to your computer is established.

- Click on "Measurement" -> "Create new measurement" in the menu bar. A dialog window opens. Here you can select the used measurement system and enter a file name for the results. Click on "Create measurements". The file will not be created before you start the measurement.

- In the menu "Measurement" you can start the recording of the measurement data by a click on "Start". All created measurements are started simultaneously. The currently measured voltages are displayed in the graph window and with their numerical values.

- To stop a measurement click on "Measurement" -> "Stop". All data recorded up to this point are saved in the file with the results.

- The measured voltages are displayed until you click on "Close new measurement" in the menu "Measurement". Then the calculated concentrations and no more the voltages are displayed.

Notes:

1) *During a running measurement (also with more than one measurement system simultaneously) you must not start an additional measurement, neither via the menu nor by a repeated call of the software. The data logger can only handle the data of one measurement process.*

2) *You should deactivate the energy saving mode of your computer, before you start a measurement. If the computer goes into the sleep mode, it will no more save any data.*

3) *In case of a sudden decrease of the measured voltages you should check, if an air bubble is trapped in the flow cell. In this case you can remove the air from the flow cell by light knocks and/or by turning around the flow cell. You can also try to intentionally transfer a bigger air bubble which you can produce by lifting the sample container through the tube. In some cases it pushes the trapped air out of the flow cell.*

5.2. Evaluation

- To evaluate a measurement open the file with the results via the menu item "File" → "Open". The file name appears in the selection list and the measured data are displayed.

- Open the corresponding dark measurement as needed. This is also displayed.

- To determine the photocatalytic activity of the sample you have to draw a straight line which fits to the measured data. First you have to select the desired measurement in the selection list.

Note:
The currently active measurement, i.e. the measurement on which any following actions like drawing a straight line, changing parameters, etc. are applied, is marked with a coloured background of the corresponding number. By a click on the file name you can select another active measurement.

- Click on "Evaluation" -> "Draw line". You can shift the line in the graph window by dragging the end points to the correct positions with the mouse (left mouse button pushed). The line's slope and the respectively calculated degradation rate are displayed with their numerical values. Once you have drawn the correct line, you can save it with a click on "File" → "Save".

- Select the dark measurement in the selection list as needed and draw a line for the dark measurement.

- In order to subtract the dark measurement from the measured data click on "Evaluation" -> "Subtract dark measurement". By doing this the values of the second measurement (dark measurement) are subtracted from the first measurement in the selection list. In addition, the subtracted values are displayed in the graph window, and the respectively calculated photocatalytic activity is displayed. There is no value in the display panel for the slope. A dialog suggests a file name for the file with the subtracted data. You can rename the file.

Note:
When you open the measurement and the dark measurement, you have to stick to the sequence described above. Please consider that in any case the second curve is subtracted from the first. The degradation rate usually has a negative sign, whereas the calculated photocatalytic activity has a positive sign (see section 8).

6. Menu items

6.1. Menu item „File"

This item includes the following options:

a) <u>Open</u>: A dialog box for the selection of a file for the results opens. The measurement values in this file are displayed as measurement points or measurement curves in the graph window. Furthermore, the file name is included in the selection list.

b) <u>Save</u>: The data which are relevant for the evaluation of the selected measurement are saved into the file with the results. The data of that measurement are saved which is marked in the selection list.

c) <u>Close</u>: The selected file with the results as well as the respective curves are closed.

d) <u>Close all</u>: A window opens where all open files are displayed which have been changed. Here you can select with a checkmark which changed files shall be saved before the program closes. If no file is marked, no changes will be saved.
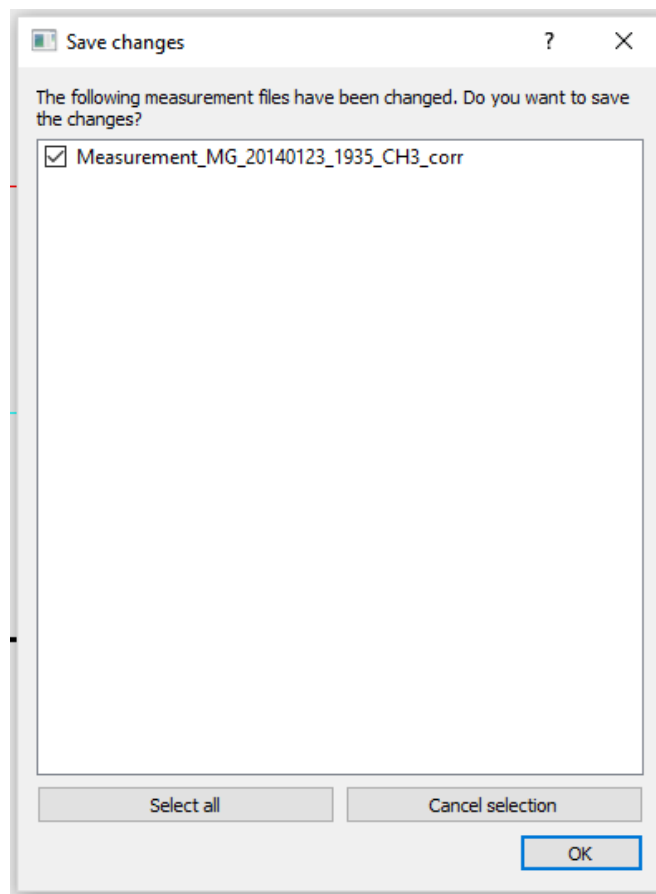

Figure 2: Selection window for saving changes.

e) <u>Exit</u>: The program is closed. If a measurement is running, a confirmation message pops up, which asks if the measurement shall be stopped and the program shall actually be closed.

6.2. Menu item "Measurement"

This item offers the following options:

a) <u>Create new measurement</u>: A dialog window opens where you can define on which channels you want to carry out a measurement. In addition you can enter the name and the directory of the file with the results. By default the software suggests the name "Measurement_[Date]_[Time]_[Channel].txt" and the directory "results".

The file with the results is prepared for the data recording by click on "Create measurements", but it is not saved on the disk yet. It is saved when you click on "Measurement" → "Start". All created measurements will start simultaneously. They are displayed in the selection list.

All curves, which are opened at this time, will be closed automatically.

The default parameters of the file "settings.txt" for the respective channel are written into the file with the results.

The measured data are visualised in the graph window. The voltages are plotted along the y axis, and in a panel. The UV light power and the temperature of the illumination chamber and, if available, the humidity are also displayed in respective panels.

All menu items except of "Stop", "Exit" and the items in "?" are deactivated.

The measurement state is set to "New measurement created (1)".

b) <u>Start measurement</u>: After the start of the measurement you can see the course of the voltages. In the first minute the values are displayed with 1 Hz, after that with 1 value per minute. The voltages are still measured with 1 Hz, but the data are averaged and saved for each period of 1 minute. For the first minute the file with the results also includes only one value.

The measurement state is set to "Measurement running (2)".

c) <u>Stop measurement</u>: By click on "Measurement" → "Stop" the current measurement is stopped. You see a confirmation dialog. The recorded data are saved.

The measurement state is set to "Measurement stopped (3)".

A message appears in the graph window that the voltages are displayed until you click on "Measurement" → "Close new measurement". Before that all menu items remain inactive.

d) <u>Close new measurement</u>: A click on "Measurement" → "Close new measurement" closes the visualisation of the voltages. Now the program switches to the display on concentrations. All menu items are active again. The displays for the slope and the degradation rate or the photocatalytic activity appear.

<u>Notes</u>:

1) *During a running measurement you can not open and process further data in the program. However, it is possible to start the program twice so that you can process data in the second copy when a measurement is performed with the first copy.*

2) *If a measurement takes less than 1 minute, no values will be saved into the file with the results. Such files are automatically deleted by the software.*

6.3. Menu item "Evaluation"

a) <u>Edit parameters</u>: Here you can enter calibration coefficients and parameter settings for the measurement (volume of MB solution, irradiated area) for a specific measurement. The values will only be written into the file with the results for this specific measurement. The default parameters are not changed (see section 6.4).
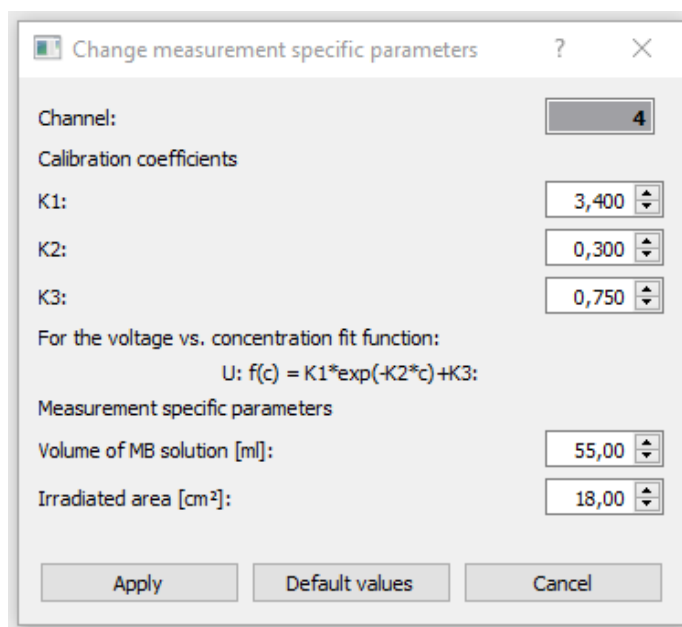

Figure 3: Here you can change the parameters for an individual measurement.
The changes do not apply to any other measurements

<u>Note</u>:
The parameter K3 must always be smaller than the lowest measured voltage in order to get a meaningful result (see the equations in section 8).

b) <u>Subtract dark measurement</u>: With this function you can subtract dark measurements from the current data. The function leads to a new file. A dialog opens which suggest a file name based on the file name of the evaluated measurement with an additional "_corr". But you can change the file name and the directory.

<u>Note</u>:
You have to stick to the described sequence when you open the measurement and the dark measurement, since always the second curve is subtracted from the first.

After subtraction of the dark measurement, if the slope of both curves is available, the photocatalytic activity (positive value) is displayed instead of the degradation rate (negative value). The indication "photocatalytic activity" of the lower panel says that it is a subtracted measurement.

You can not carry out further actions on parameters of the subtracted measurement.

<u>Note</u>:
The file with the results includes as many values as the measurement with the lower number of values, i.e. with the shorter measurement time.

c) <u>Draw line</u>: Here you can draw a fit line which slope is used to calculate the degradation rate and the photocatalytic activity of the sample. The coordinates of the line are written into the file with the results if you click on "Save".

6.4. Menu item "Configuration"

<u>Default parameters</u>: Here you can define default parameters for the calibration of each channel. These parameters are saved in the file "settings.txt". If you create a new measurement, these default parameters are used (as long as you do not define specific values for the measurement).
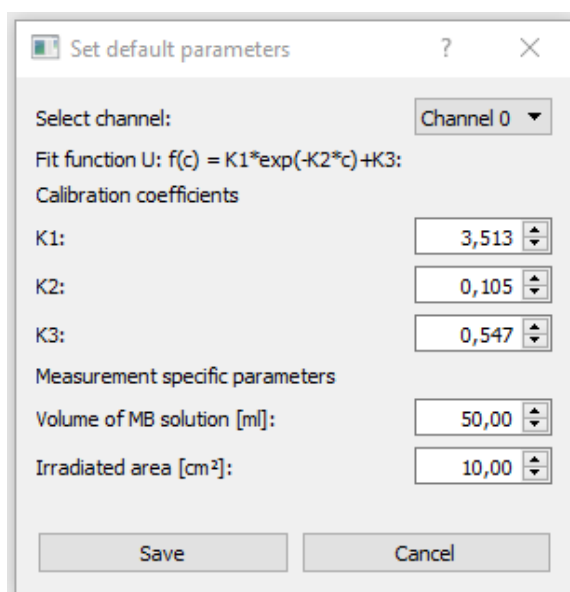

Figure 4: Here you can enter default parameters. They are applied in all following measurements.

6.5. Menu item "?"

Here you find the user manual as well as information on the *PhotoKat* software version and the vendor.

6.6. Context menu of graph window

By holding the left mouse button in the graph window you can obtain a cross-hair and the coordinates.

By pressing the right mouse button in the graph window you can open a context menu which contains the following items:

a) <u>Scale axes</u>: Here you can manually change the scaling of the x and y axes. This function can be helpful for the evaluation. The changed scaling can not be saved. (The item is only active if the mouse pointer is close to an axis.)

b) <u>Connect points</u>: This function connects the measurement points to a line.

c) <u>Zoom:</u> After a click on "Zoom" you can drag a rectangle in the graph window to obtain an enlarged view.

d) Scale automatically: This function scales the x and y axes automatically considering the currently selected measurement curve. The manual scaling (a) and the zoom (c) can be reset by this function.

Note:
During a running measurement only the item "Connect points" is applicable. The other items in the context menu are deactivated.

7. Calibration

To calculate the methylene blue concentrations from the measured voltages the software makes use of the following calibration functions:

(a) $U_t = K1 * \exp(-K2 * c_t) + K3$ [1] and its inverse function

(b) $c_t = \ln((U_t - K3) / K1) / (-K2)$ [2]

The function (a) represents the fit curve according to Levenberg-Marquardt. Figure 5 shows the system specific calibration curve carried out and used by MRC. MRC's default values of the calibration coefficients stored in your software for the different channels are:

	Channel 0	Channel 1
K1	3,61468	3,68072
K2	0.101704	0,0971813
K3	0.614568	0,55502

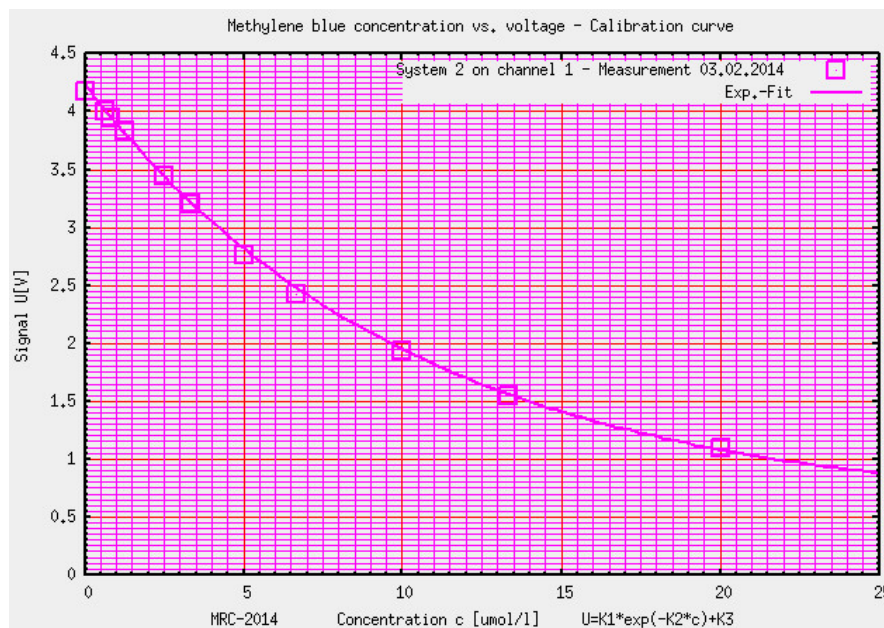The concentration c_t corresponding to a measured voltage U_t is calculated with equation (b).

Figure 5: Calibration curve: methylene blue concentration [µmol/l] vs. measured voltage [V].
It is used to determine the calibration coefficients for the measurement system

By changing the calibration coefficients you can carry out a recalibration if the conditions have changed so that the initial U/c correlation is no more valid.

8. Stored equations for the evaluation of data in the software

Measured and saved data can be evaluated according to the standard DIN 52980. The following equations are used for this purpose.

With the equation for the specific degradation rate

$$R = \Delta A_\lambda \cdot V / \Delta t \cdot \epsilon \cdot d \cdot A \qquad [3]$$

and Lambert-Beer`s law

$$A_\lambda = c \cdot \epsilon \cdot d \quad \rightarrow \quad \Delta A_\lambda = \Delta c \cdot \epsilon \cdot d \qquad [4]$$

the specific degradation rates with (R_{irr}) and without (R_{dark}) illumination can be calculated:

$$R = dc/dt \cdot V / A \qquad [5]$$

dc/dt: Slope of the concentration over time [µmol/l*h]

V: Volume of the solution [l]

A: irradiated area [m²]

The specific photocatalytic activity can then be determined as the difference between the specific degradation rates R_{dark} and $R_{irr:}$:

$$P_{MB} = R_{dark} - R_{irr} \qquad [6]$$

Note:
The displayed degradation rate has a negative sign, since usually the concentration decreases over time, so that dc/dt in equation [5] is negative. The calculation of the photocatalytic activity according to equation [6] leads to a positive sign of the activity, since R_{dark} is usually less negative than R_{irr}.

9. Format of data in the file with the results

Since the read-out of the file with the results takes place sequentially, it must always have the structure as described below. If the format of the file does not match this structure, an error message "Invalid data format" is displayed.

The file includes the following data: Date and time of the measurement's start, state, channel, parameters, degradation grade or photocatalytic activity, coordinates of the line, and – in tabular form for each measurement point – a consecutive number, the time, concentration, concentration of dark sample, light intensity, temperature, relative humidity, and the measured voltage.

By the subtraction of the dark measurement a new file is created where the values of the illuminated and the dark samples are set off against each other. This corrected file has the same format as described above. Now it includes the corrected concentrations in "C" which result from the subtraction of the values of the dark measurement. In addition, "DS" shows the concentration of the dark sample.

```
*********************************************************************
*Measurement start: 2013-04-25T16:24:50        State: 5   Channel: 1
*Parameters: 5.513 0.105 0.547 50 10  R/P: -6.995
*Slope: 0.0000 0 0.0000 0
*No.    Time           C      DS     UV     T      RH     V
*********************************************************************
1      16:25:50 9.31    5.76   0.00   0.00   0.00   1.68
2      16:26:50 9.16    5.58   0.00   0.00   0.00   1.72
3      16:27:50 9.16    5.58   0.00   0.00   0.00   1.72
4      16:28:50 9.27    5.72   0.00   0.00   0.00   1.69
5      16:29:50 9.16    5.58   0.00   0.00   0.00   1.72
6      16:30:50 9.19    5.63   0.00   0.00   0.00   1.71
7      16:31:50 9.23    5.67   0.00   0.00   0.00   1.70
8      16:32:50 9.12    5.54   0.00   0.00   0.00   1.73
9      16:33:50 9.39    5.85   0.00   0.00   0.00   1.66
10     16:34:50 9.12    5.54   0.00   0.00   0.00   1.73
11     16:35:50 9.16    5.58   0.00   0.00   0.00   1.72
12     16:36:50 9.19    5.63   0.00   0.00   0.00   1.71
13     16:37:50 9.27    5.72   0.00   0.00   0.00   1.69
14     16:38:50 9.39    5.85   0.00   0.00   0.00   1.66
15     16:39:50 9.19    5.63   0.00   0.00   0.00   1.71
16     16:40:50 9.34    5.81   0.00   0.00   0.00   1.67
17     16:41:50 9.19    5.63   0.00   0.00   0.00   1.71
18     16:42:50 9.27    5.72   0.00   0.00   0.00   1.69
19     16:43:50 9.39    5.85   0.00   0.00   0.00   1.66
20     16:44:50 9.16    5.58   0.00   0.00   0.00   1.72
21     16:45:50 9.31    5.76   0.00   0.00   0.00   1.68
22     16:46:50 9.39    5.85   0.00   0.00   0.00   1.66
23     16:47:50 9.34    5.81   0.00   0.00   0.00   1.67
24     16:48:50 9.39    5.85   0.00   0.00   0.00   1.66
25     16:49:50 9.31    5.76   0.00   0.00   0.00   1.68
26     16:50:50 9.42    5.90   0.00   0.00   0.00   1.65
```

Figure 6: Example of a file with the results after subtraction of a dark measurement

Hereinafter the entries in the file are explained:

a) State: 1= New measurement created, 2 = Measurement running, 3 = Measurement stopped, 4 = Measurement loaded for evaluation; 5 = Dark measurement subtracted

b) Channel: Number of the channel where the measurement took place.

c) Parameters: K1, K2, K3 (for calibration), volume of test solution [ml], illuminated area [cm²]

d) R/P: Degradation rate (negative value) or photocatalytic activity (positive value) [µmol/m²h]

e) Slope: Coordinates y_1 [µmol/l] | x_1 [sec] | y_2 [µmol/l] | x_2 [sec]

f) No..: Consecutive number for each entry in the table

g) Time: Time stamp of each entry in the table

h) C: Calculated methylene blue concentration [µmol/l] for each measurement value. In files where the dark measurement was subtracted, the concentration reduced by the dark measurement is inserted here

i) DS: Calculated concentration of the dark sample [µmol/l]. Before the subtraction of the dark measurement in the evaluation 0.00 is inserted here.

j) <u>UV</u>: UV light intensity [mW/cm²]

k) <u>T</u>: Temperature [°C]

l) <u>RH</u>: relative humidity [%]

m) <u>V</u>: Averaged voltages [V] measured by the transmission measurement system. The measurement takes place with a rate of 1 Hz, the inserted values are averages over 1 minute. These voltages are used to calculate the MB concentrations considering the calibration.

10. Error messages

„Invalid device number (837)":
The USB cable is not connected. Please check the USB connection to your PC or laptop.

„Invalid device number (838)":
Wrong serial number of the data logger. Please check if the right data logger according to your software licence is connected.

„Invalid data format":
The format of the file with the results was altered, or the measurement was stopped within the first minute. The file can not be read. Please correct the file format, if necessary, to the format described in section 9.

11. Contact

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12. Appendix

12.1. Used formula symbols and units

U	Voltage	[V]
ε	Molar extinction coefficient	[m²/mol]
t	Time	[h]
t_m	Measurement time	[h]
c_t	Methylene blue concentration	[mol/l]
A_λ	Absorbance	[1]
d	Measurement distance	[mm]
V	Volume of solution	[l]
A	Irradiated area	[m²]
λ	Wavelength	[m]
E	Irradiation power	[W/m²]
R	Specific degradation rate	[μmol/(m²h)]
P_{MB}	Specific photocatalytic activity	[μmol/(m²h)]
dc/dt	Slope of straight line	[μmol/l h]

12.2. Procedure to import data into other programs

It is generally recommended to work with a copy of the file with the results if it is imported into other programs like Microsoft Excel. In that way you can avoid that the file format is accidentally altered so that the *Photokat* software can no more read it.

For the import into Excel you can go to "File"->"Open", select "Text files" from the "Open" dialog box, and select the text file that you want to open. Depending on the Excel version, a wizard should appear where you can first select "separated" or "delimited". In a second step you have to select "tabs", "treat consecutive delimiters as one". In the final step you might have to select "." as the decimal separator and " " (empty) as the thousands separator. The data should then be imported with "Complete".