Airyx SkySpec Instrument (MAX-DOAS) Instruction Manual (preliminary)

Airyx GmbH, Justus-von-Liebig Str. 14, 69214 Eppelheim / Heidelberg, Germany

January 8, 2018

Contents

0.1 Safety Guidelines

Before installation and operation of the instrument read the safety guidelines carefully.

The instalation, assembly and operation of this instrument is only allowed by trained technicians and experts who are familiar with the correct operation and handling due to their education and expertise. If you are unsure with any of the technical procedure enquire your technical support or the manufacturer for assistance. Do not try any unclear procedure.

The instruments are only allowed to be operated in the desired manner. The use and operation has to be done carefully. Incorrect use may damage or destroy the instrument, result in bad measurement data and may be a risk for people and the environment. Any modification is not covered by the manufacture.

0.1.1 Installation

For the installation and operation consider:

1. Follow exactly the instruction
2. Use only original parts from the manufacturer
3. Only provided power supplies are allowed
4. The instruments are supposed to be used on solid ground.
5. The location for the indoor components is not allowed to be dirty, dusty, with extreme heat and cold, high humidity, strong electromagnetic radiation or strong light radiation.
6. If the scanner is installed on top of a building, take care of sufficient lightning protection.
7. Keep the instrument clean.
8. Materials, liquids or gases which are easily inflammable, explosive, alkaline or acidic have to be kept away from any parts of the instrument.
9. Damaged instruments are not allowed to be operated. Stop immediately the instrument and remove the power line.
10. If you observe extreme heat production of the instrument immediately stop it and remove the power line. First ensure that the instrument is not damaged before starting it again.
11. To clean, maintain and repair the instrument wear always protective gloves.
12. If operating UV light sources like mercury calibration lamps, always wear appropriate protective googles. UV light may damage your eyes up to blindness.
13. Operate and handle the instrument always with care as appropriate for any sensitive scientific instrument.

0.1.2 Transportation

Transportation has to fulfil:

1. Carefully disassemble the instrument. First turn off the instrument and remove the power line. Remove the fibre and then the cables if necessary.
2. Cover the sensitive optics with adequate protection
3. Place the instrument in a robust transport box

4. Place sufficient packing material around the instrument to prevent any damages during all transport conditions.
5. Avoid high humidity and water entering the transport box, eventually use additional desiccant.

Chapter 1

Introduction

This document describes the setup routine for the instrument as well as for the accompagning measurement software MS-DOAS by Udo Frieß.

1.1 Properties of Airyx SkySpec instruments

1. Multi Axis (MAX) - DOAS System for measurements of atmospheric trace-gases
2. One or two ultra-low straylight 75mm Avantes spectrometer
   - e.g. UV: 295 – 450nm, 100 μmm slit (from fibre), 0.6nm resolution, Hamamatsu backthinned detector optimized for UV, Schott BG3 filter
   - e.g. Visible: 430 – 565nm, 100 μm slit (from fibre), 0.6nm resolution, Sony 2048L detector

   Typical instrumental stray light $< 0.05\%$, RMS of $1 \cdot 10^{-4}$ (vis) and $2 \cdot 10^{-4}$ (uv) for ≈ 1000 scans around noon.
3. Temperatur stabilization of both spectrometers at a fixed temperature with a deviation of $< 0.05°$C
4. Inclination measurements inside the scanning head to simplify installation and measurement routine, allows automatic elevation adjustment.
5. Elevation angle accuracy $< 0.1°$
6. Telescope field of view (opening angle) $< 0.3°$
7. Telescope scanner unit is sealed, weatherproof and heated to avoid icecover at low temperatures
8. Telescope scanner unit covers elevation angles from -10°-180°
9. Ambient temperature and pressure measurements
10. Optimized light efficiency for high measurement quality

Chapter 2

Mechanical Setup and Installation

The instrument consists of two main units: The telescope scanner unit and the spectrometer unit, which also incorporates the temperature stabilization of both spectrometers, USB communication and control-electronics for additional sensors for temperature, pressure, inclination and the telescope elevation stepper-motor.

All external plugs of the setup are chosen in such a way that it can be only connected if the right connectors are chosen. This avoids errors during setup and simplifies the setup process.Still, if you have several spectrometer boxes and telescope units, only use the correct pair together. The telescope units have been calibrated and the settings are stored in the micro-controller within the spectrometer unit. Exchanging telescopes might lead to incorrectly measured elevation angles.

2.1 Spectrometer Unit

Both spectrometers are temperature stabilized and are located within the box shown in Figure 2.1. Since the highly sensitive spectrometers are sensitive to humidity, the only connection for ambient air from the outside to the inside of the instruments leads throught a tube filled with humidity absorbing silica gel. This connection is necessary to compensate for changes in ambient pressure. To be sure that the air inside the box is dry and does not cause condensing water on the spectrometers, a package of silica gel can also be found within the spectrometer unit box.

Do not disconnect the fibres in the spectrometer box, they are carefully adjusted!

2.1.1 Installation

1. Locate the spectrometer box in a lab in a way that the cables and the fibre at the front have sufficient space and the fibre cannot be accidently damaged

2. Connect the power supply with the power plug to the spectrometer box

3. Connect the USB cable to the Computer. The USB connector is neither airtight nor waterproof, if the specially designed connector cable to the PC is not plugged in and fixed. If you need a longer USB cable, extend the existing cable instead of replacing the USB cable included with this instrument or order a longer cable (Type Bulgin PX0840 up to 5m). If the USB is not connected, make sure to close the plug with the attached cap. All other connectors are airtight.

After connecting the power plug and the USB connector, the telescope scanner unit needs to be attached to the spectrometer unit. Due to unique plugs, it is not possible to connect them in a wrong way. If a plug does not fit, check again the orientation of the plug and the number of pins of both the plug and the connector.

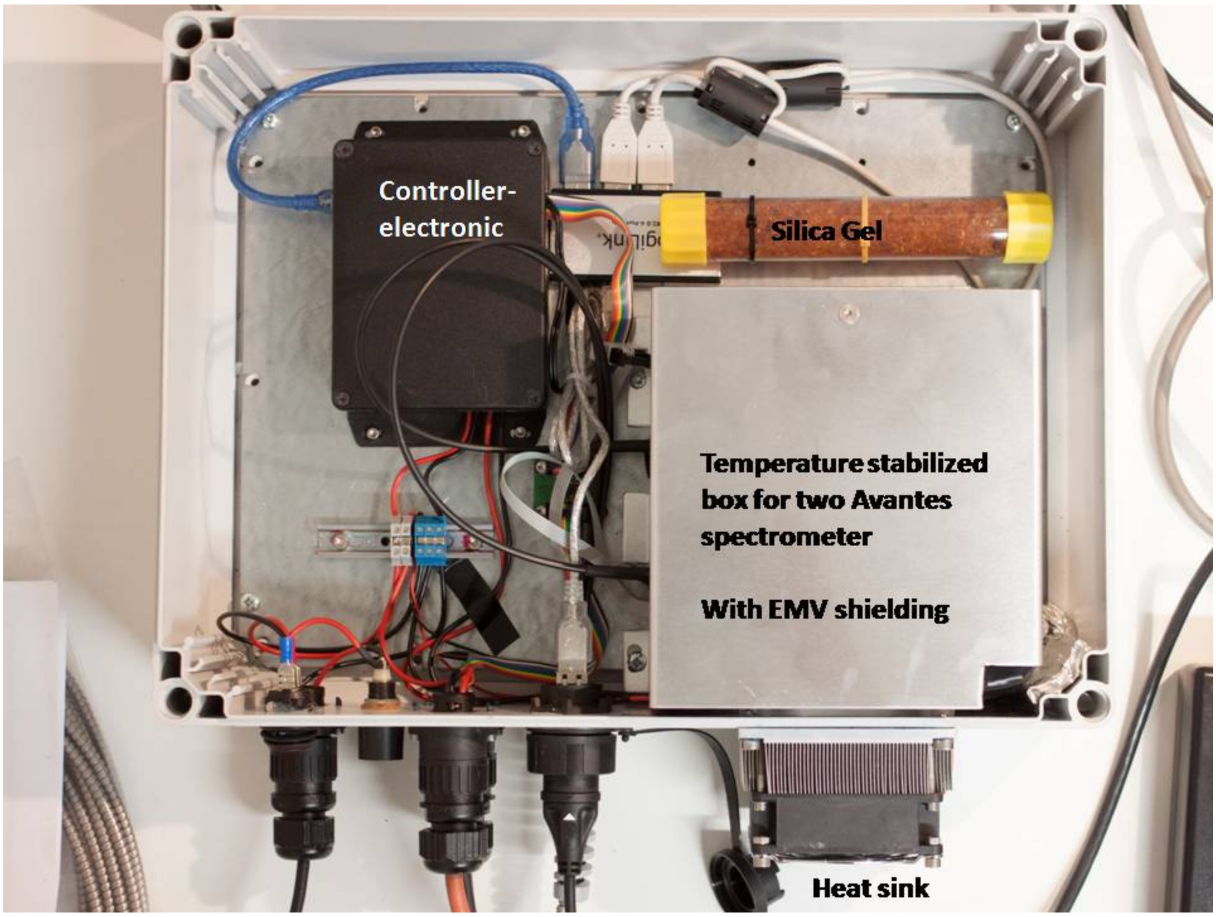


Figure 2.1: Airyx SkySpec spectrometer box

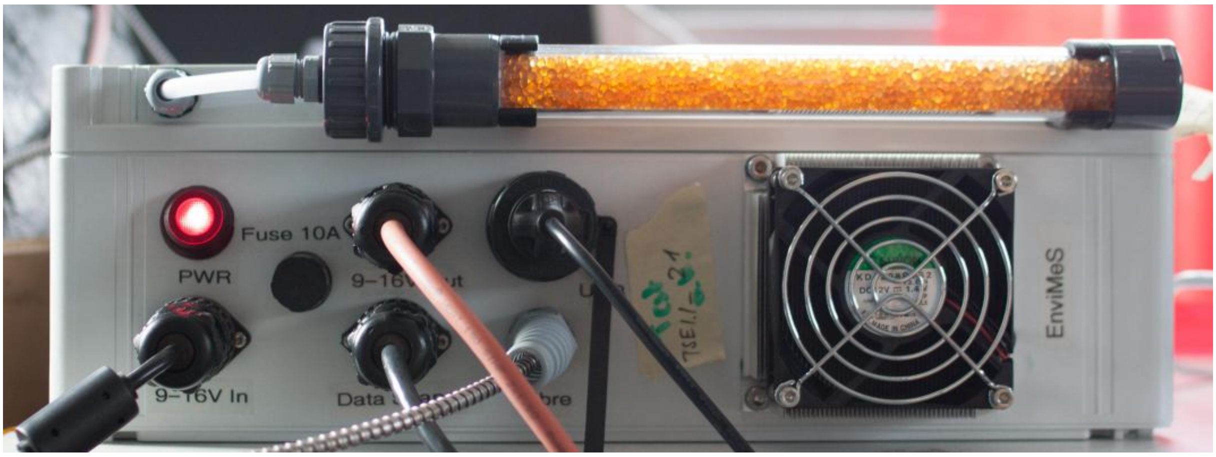


Figure 2.2: The front of the spectrometer box. From left to right: Power switch, power connector, 10A fast fuse, 9-16V power supply telescope scanner unit, data cable for scanner, airtight USB connector to computer, fibre, heatsink. On top is a tube of desiccant, which should be changed when the color has changed from orange to green and blue entirely.

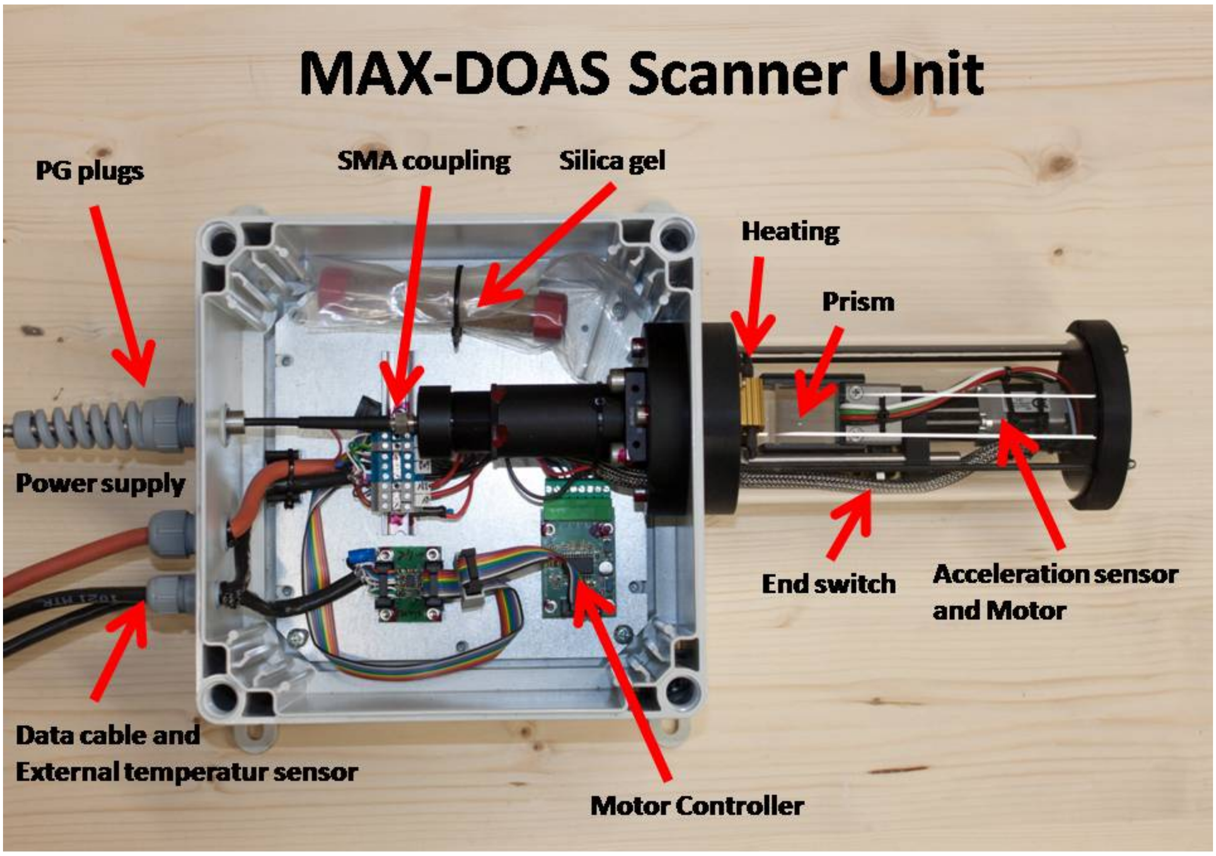


Figure 2.3: The 1D telescope scanner box.

If you have two spectrometer boxes and one or more telescope scanner unit, always connect each of the scanner units to only one of the spectrometer boxes each! Connect both cables to the same spectrometer box!

2.2 Telescope Scanner Unit

The 1D-telescope scanning unit is shown in Figure 2.3. It consists of the motor, electronics, the MEMS inclination sensor and the optical parts: A quartz-glass tube to protect the rotating prism which reflects the light through a lens onto the fibre at the end of an adjustable tube. This setup allows the user to collect light from a defined elevation angle from a vertical opening angle of approximately 0.2 ° to be spectrally analysed in the spectrometers.

The 1D-telescope can additionally contain a shutter and a mercury emission lamp in order to record calibration spectra even under sunlit conditions.

The Airyx SkySpec-2D telescope has a almost identical Airyx SkySpec-1D telescope scanning unit on top of an azimuth motor. The Airyx SkySpec-2D telescopes are often equipped with a diffuser element in order to allow for direct sun measurements and can contain a mercury emission lamp.

2.2.1 Installation

1. Mount the telescope scanner box upright on a fixed wall or mounting, with a free line of sight towards the horizon as well as straight upwards to zenith. At the four corners of the scanner box mounting clips are located outside of the box. Chose a suitable azimuth viewing direction to avoid measurements directly into the sun or close to the sun at all possible measurement days. The telescope collects light from the direction of the removable lid of the scanner telescope box. Make sure the scanner is mounted vertically. Deviations from the ideal position along the rotation axis of the telescope will be compensated by the inclination sensor.

2. Open the scanner unit and then the PG-Plug on the outside of the box.

3. Lead the fibre first throught the plug and then carefully into the Telescope Scanner Unit (see also Figure 1)

4. **Make sure that the rubber sealing is tight on the fibre stainless steel tubing and placed finally within the PG-plug.** (see also Figure 4)

5. Remove the fibre protection cap and connect it to the fibre connector at the end of the black tube using the SMA-connector.
   Make sure that the fibre is neither strongly bent nor torn, this can destroy it. **Do not move any of the optomechanic components, they are precisely adjusted.** (see also Figure 3)

6. Tighten also the PG-connector at the outside of the scanner box - this also seals the entrance of the fibre from the outside. (see also Figure 5)

7. Before closing the scanner box again, open the plastic bag with silica gel to absorb the remaining water vapor within the scanner. This should keep the scanner free from condensed water and you can increase the lifetime of the silica gel by placing more silica gel in the scanner box.

8. Since this instrument is based on measuring absorption using UV and visible light from the sun, make sure that the instrument is not exposed in an unnecessary way to dirt and dust to keep the quartz cylinder as clean as possible. Clean it with water and a soft tissue if necessary.

2.2.2 Telescope Scanner Unit with calibration lamp and shutter

The version of the Telescope Scanner Unit with calibration lamp and shutter allows you to record offset and dark current spectra as well as mercury discharge lamp spectra automatically. An example how this can be done can be seen in the *RecCalibration* script and is also included in the measurement script.

2.2.3 Airyx SkySpec-2D Telescope Scanner Unit

To allow for measurements at different azimuth angles, the Airyx SkySpec-2D telescope scanner unit is a Airyx SkySpec-1D unit extended by an azimuth motor. The shutter and calibration lamp are replaced by a diffuser to allow for direct sun measurements. (see Figure 9)

2.3 Maintenance

- **Cleaning of optics:** Whenever the quartz cylinder is dirty, it can be cleaned with water. Depending on the measurement site, this might be a necessary daily routine e.g. at marine sites with sea spray.

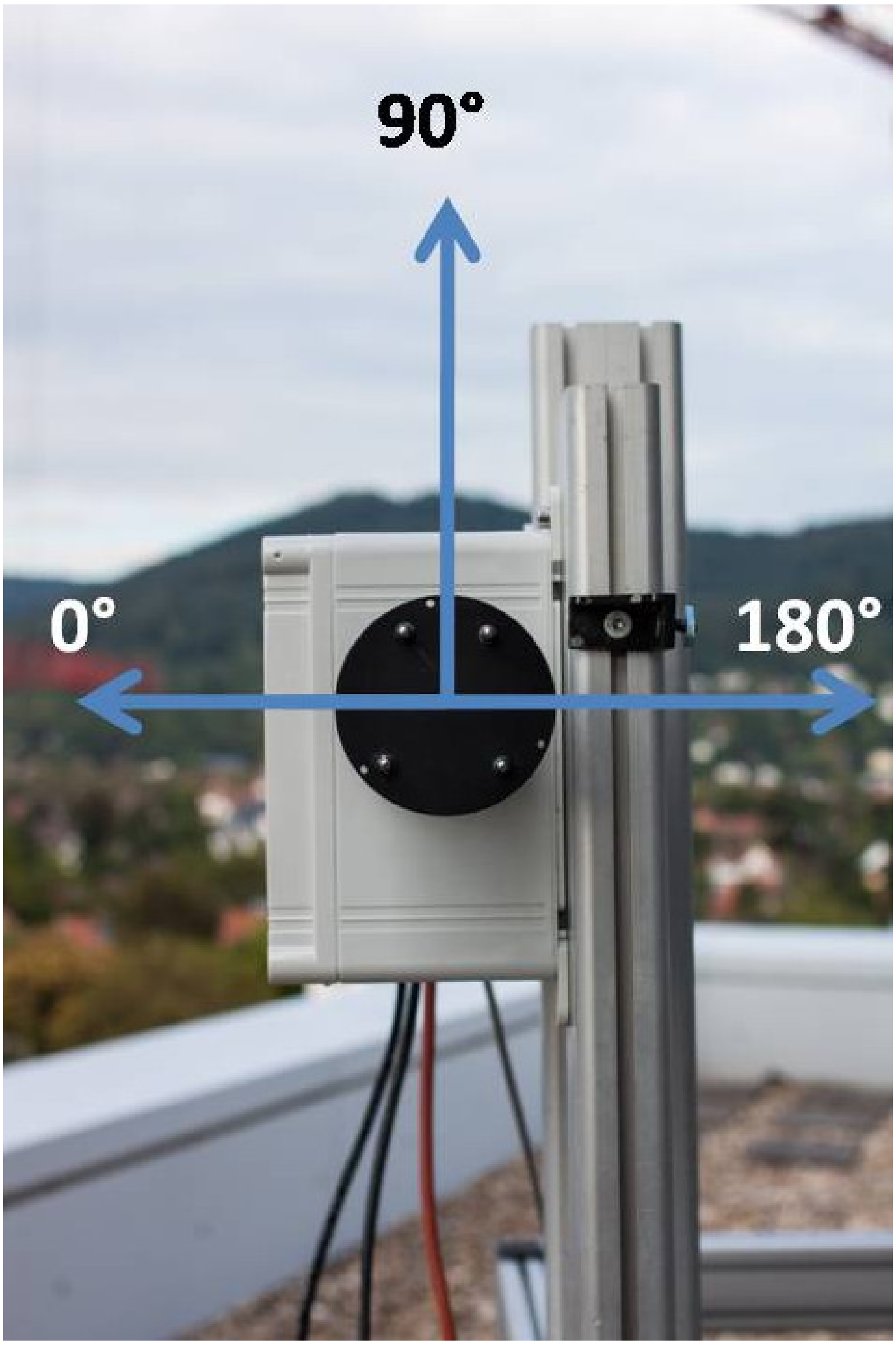


Figure 2.4: Telescope elevation angles of the scanner box.

- **Desiccant:** The telescope scanner unit and the spectrometer box contain desiccant to absorb humidity within the instrument. For the telescope scanner box the silica should be checked every three month. Depending on the condition of the silica gel this period needs to be shortend or can be extended. The lifetime can be also extended by using more silica gel. For the spectrometer box an inspection is only needed once the outside tube has changed its colour from orange to green. Then the content of the tube needs to be replaced and an inspection of the silica gel located within the box might be necessary. The silica gel can be used again after it has been heated to 130 °C for at about 24 hours until the desiccant is orange again [1]. If you use own desiccant this is also depending on the information given by the manufacturer of the silica gel in use.

- **Dust cleaning:** The fan and the heat sink of the temperature stabilization of the spectrometer unit need to be cleaned from dust, if necessary.
- **Telescope elevation alignment:** The telescope elevation angles are calibrated before shipping the instrument in the lab. However, if the optical parts of the instruments are modified, it is crucial for final data evaluations to test the elevation calibration of the instrument again. Such modification can happen intentionally or unintentionally, e.g. if the telescope fell onto the ground during installation or transportation.

  Therefore the telescope elevation calibration should be monitored regularly during operation. During long-term measurements and measurement campaigns (MADCAT, CINDI-2, ...) often the first two options are applied, method 3 is suitable for tests before and after measurement campaigns.

  1. A point light source can be placed in a distance of typically more than 10 m from the MAX-DOAS telescope. The height of the lamp needs to be adjusted using a (laser-) level to the height of the telescope head. Then the intensity can be measured at different telescope positions (see e.g. the 'horscan' script in the MSDOAS project: This script iteratively records the received intensity at different elevation angles). Plotting the intensity values over elevation then shows if the telescope has an elevation angle offset.
  2. The (natural) horizon can be scanned similarly as in 1), if it is not blocked by buildings and/or trees. The derivative of the intensity values with respect to elevation angle provides a good estimate for the FOV.
  3. A light source can be connected via a fibre to the telescope - then the image projected by the telescope can be observed on a distant screen. This requires a bright light source (such as a high power LED) and a dark lab.
  4. Both, the position as well as the shape of the field of view of the instrument can also be determined from simultaneously recorded images and MAX-DOAS data using the method presented in [Sihler et al., 2016]. This typically requires a camera providing intensity values proportional to intensity. This is often not the case for webcams, but DSLRs provide e.g. raw output files.

  All of these methods can be applied to the telescope unit at different temperatures in order to check if the elevation sensor shows a temperature dependence. As the telescope head heats up noticeably in direct sunlight, e.g. horizon scans in the morning and at noon can quantify this effect. The telescope temperature is also found in the output variables of the TSE unit.

2.4 Instrument with an embedded PC

Some of the instruments have an internal PC to run the measurements and preliminary analysis scripts, these are typically called 'SkySpec-mini'. They are the compact version of the SkySpec instruments and have only one spectrometer. If your instrument is one of these, you can either connect to the internal PC via WLAN or LAN. If you want to connect via a wireless connection, make sure that the access point in the instrument is switched on (you find a switch on the backside of the instrument). The PC is preconfigured to run a VNC server. You can connect to this server using a VNC client of your choice, e.g. TightVNC, to access the desktop of the PC remotely. In case of unknown behaviour, which cannot be diagnosed from a remote connection, the instrument comes with an adapter, which allows you to display the embedded PCs output directly on a screen (compare Figure 8). Furthermore you will find free USB slots inside the instrument to accommodate USB plugs for a keyboard and a mouse.

---

[1] This is the procedure described by the manufacturer of the desiccant included with the instrument

Note: For car measurements with the SkySpec-mini, please note that the driving direction should be the direction in which the webcam points: It should not be the direction of the fan, the switches and the cable connectors. These are waterproof, but the water pressure of heavy rain during driving could still damage the instrument.

2.4.1 Network settings for instrument with an embedded PC

LAN

For direct PC communication (LAN between 2 PCs), the LAN adapter of the embedded PC is configured as follows:

```
IP: 192.168.1.1
Submask: 255.255.255.0
```

To connect via LAN, you need to change the IP V4 settings of the LAN adapter of your PC to the following settings:

```
IP: 192.168.1.2
Submask: 255.255.255.0
```

Then you can setup a VNC connection to the embedded PC using the following setttings using a VNC client of your choice:

```
with IP  192.168.1.1
Passwd: maxdoas
```

WLAN

For direct PC communication (Wireless LAN between 2 PCs), the WLAN adapter of the embedded PC is configured as follows:

```
WLAN network maxdoas1 WPA2-PSK TKIP
channel1
Passwd: maxdoas1
```

To connect, search for available WLAN access points and connect to *MAXDOAS1*.

Then use a VNC client and use the following settings:

```
IP  192.168.100.1
Passwd: maxdoas
```

If you run your instrument with an internet connection and you know its IP address, you can also connect to your instrument over the internet.

Chapter 3

Software Installation

3.0.1 Minimum system requirements

- Microsoft ® Windows ® System newer than Windows ® 2000
- One free USB 2.0 port
- 1Ghz 32bit CPU
- 512MB RAM
- 100MB free harddisk space + measurement data storage (max. 25MB/day)

Please make sure to switch off Windows energy saving modes before starting your measurements to ensure continuous operation of the instrument.

3.1 Software and Driver Installation

The drivers for the software can be found on the CD accompagning the instrument in the folder 'drivers'.

1. The Avantes ® spectrometer drivers are installed by executing *drivers/Avantes Spectrometer Driver/setupAvaSoft* After having restarted the computer, the Spectrometers can be found in the device manager [1] of windows, see Figure 3.1. To check this driver installation, you can use AvaSpec as described in section 3.2.
2. If asked by the operating system for drivers for the FTDI chip or if you cannot connect to the control electronics and you cannot find an associated USB COM port in the system's device manager, a setup file and the extracted driver files can be found in */drivers/FTDI*. Some operating system already have these drivers included and will not ask for them.
3. Extract the zip file from the MS-DOAS folder on the CD and point to a folder to which you would like to install the program. The measurement program MS-DOAS for which the purchase of this instrument also included a license for non-commercial use can be found in this folder after completing the installation. Also a configuration file called *'Sky SerialNumber.mmp'* can be found in this folder and can be loaded by MS-DOAS. If you do not want to start the script right away, stop all devices (red circle below the menu, top-left corner).

For necessary settings in MS-DOAS during setup, see subsection 4.1.1.

---

[1] **Windows 7:** press the start orb on your screen and then type 'device manager' into the search box. **Windows 2000/XP:** Press start, then Settings, Control panel, and finally 'Systems'. There you need to select the 'hardware' tab where you find a button to get to the device manager.

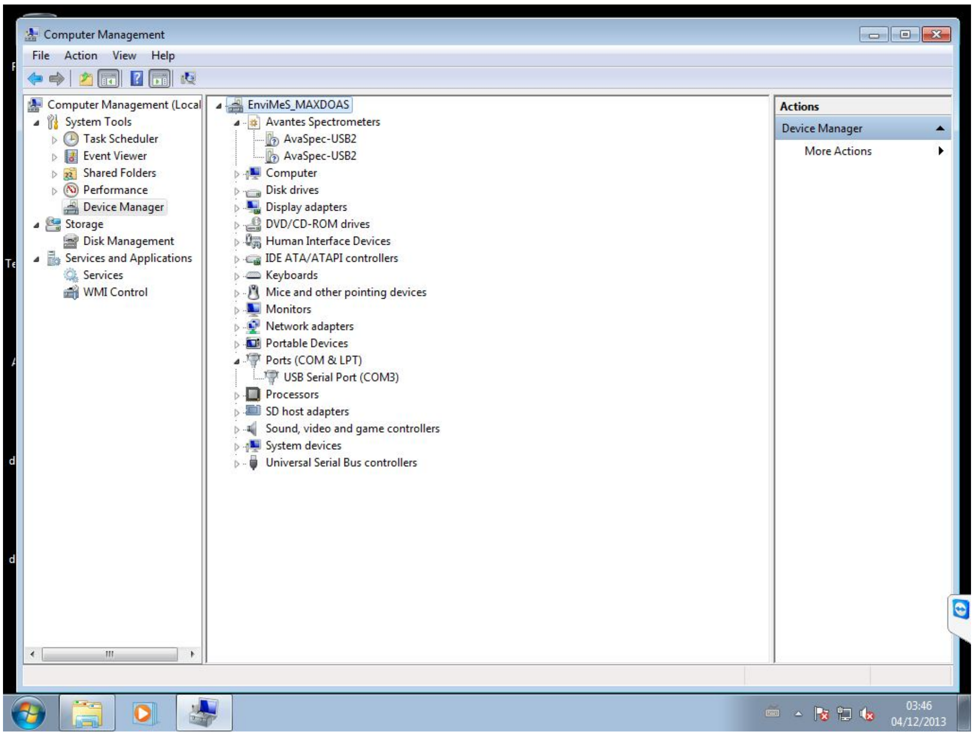


Figure 3.1: Two Avantes Spectrometers can be found in Windows 'device manager' after installation. Further below, also the COM port which is used for communication with the TSE board can be found.

3.2 Testing the spectrometers with Avaspec

Avantes, the manufacturer of the spectrometer, also delivers a program with which spectra can be recorded. It is included within the driver package and can be found after installation in the start menu *Programs/Avantes Software/AvaSoft 7.7 for AvaSpec-USB2.* **For the normal measurement routine, this program is not needed.**

If the drivers and the spectrometer itself is properly installed, you should be able to record spectra with this software and see e.g. sunlight spectra as shown in Figure 3.2. If this is not the case and e.g. no spectrometer can be found, check all connections and reinstall the driver software.

```
UV - 1301206U1
Auto - fixed tin  TExp: 82  TTot: 60000  Sat: 70
TAcq:  50351.5 Scans:   610   Max: 6983838 Min:  120266 Avg: 4074492 Name:   File:
SZA:  37.53  SAA:  186.12  LZA:  139.68  LAA:  19.99  LPH:  94.8%  21.08.13 11:43:23

Vis1 - 1212142U1
Auto - fixed tir  TExp: 54  TTot: 60000  Sat: 70
TAcq:  47980.2 Scans:   892   Max: 10208998 Min:  566914 Avg: 474089 Name:   File:
SZA:  37.53  SAA:  186.12  LZA:  139.68  LAA:  19.99  LPH:  94.8%  21.08.13 11:43:23
```

```
21.08.2013 11:36:07 AM  Connection to Avantes Spectrometer 1212142U1 established.
21.08.2013 11:36:11 AM  Connection to Arduino established.
21.08.2013 11:36:13 AM  Connection to Arduino Stepper  established.
21.08.2013 11:36:25 AM  "Starting Measurement in 30 Seconds..."
Comment:
SZA:  37.89  SAA:  191.86  LZA:  138.79  LAA:  24.98  LPH:  94.9%  LAT:  49.50  LON:   8.66      21.08.2013 11:58:16 AM
```

Figure 3.2: This is how the Avantes Avaspec Software should look like if both spectrometers have been detected.

Chapter 4

Software Description

MS-DOAS by Udo Frieß is used for controlling the instrument and processing the measurement data.

4.1 MSDOAS - Measurement software

MS-DOAS has been developed by Udo Frieß and is restricted **to non-commercial use only**. Individual licenses for commerical use can be purchased. When starting up, an empty screen with a menu will be seen. For the Airyx SkySpec (MAX-DOAS) instrument a configuration file has been prepared (*'Sky SerialNumber.mmp'*) which can be found in the MS-DOAS folder. After having selected to load this file from the menu, the screen looks like in Figure 4.1. The window on the left side contains the available devices, such as physical devices, but also logging files and controlling scripts. Among the devices the measurement script can be found and, if needed, manually started. TSE (Temperature and Stepper Motor Electronics) has two subdevices, one of them is the elevation motor, the other one the temperature controller.

If you have multiple instruments, do not use a similar config file with the wrong serial number for your instrument! Even though most instrumental parts might work, the cooling parameter might differ for different instruments, and therefore the temperature control of the spectrometers might not work properly.

UV and *Vis1* are the two spectrometers implemented in this SkySpec (MAX-DOAS) instrument. When no script is running, you can manually record spectra after setting integration time, scan number and total time for the measurement by clicking on the lightbulb for a single measurement or on the clock for continuous measurements.

The script *'startup'* is executed after loading the MS-DOAS project and is normally used to immediately start up initialization processes and then the measurement script itself. To disable it, remove it or rename it.

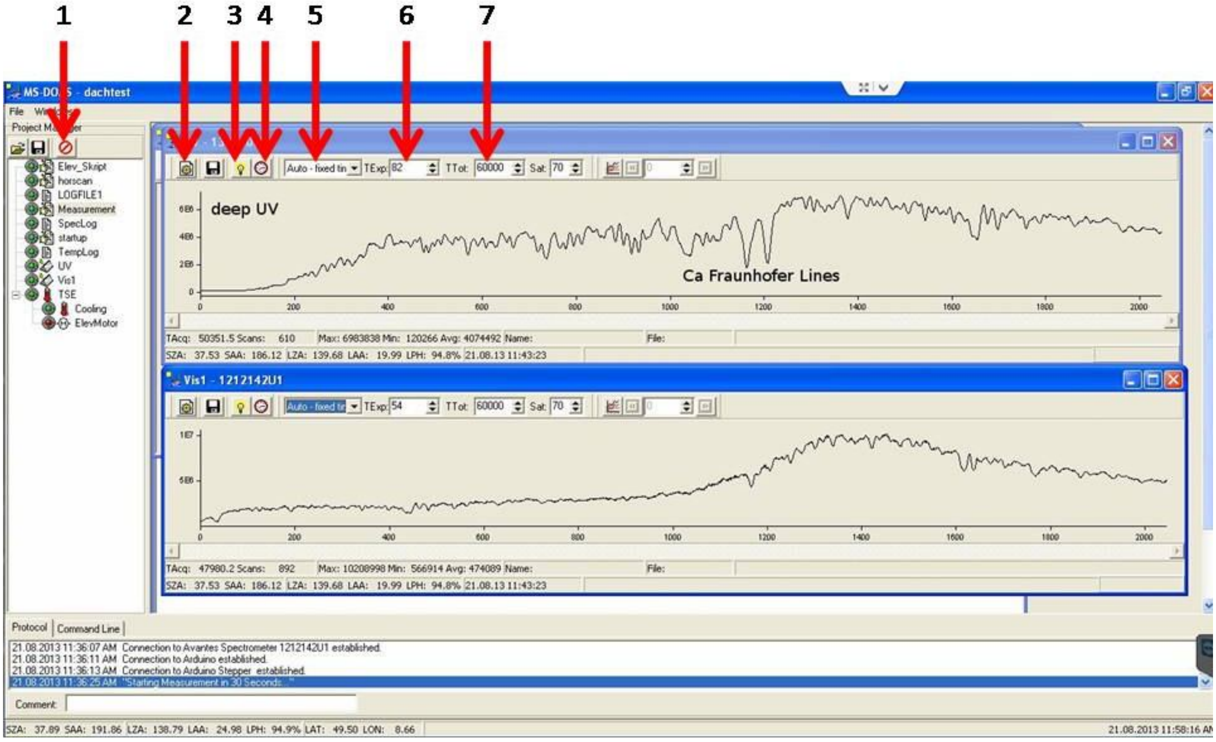
MS-DOAS comes with a short introduction to its scripting language, which can also be found in the installation folder, called *'A short introduction to scripting.doc'*.

4.1.1 First start of MS-DOAS

Typically, the MS-DOAS projects are set up in a fashion that the measurement script is started automatically. This simplifies the start of measurements when a link to MS-DOAS and the respective project file had been places in Windows(R) startup folder. If you don't want the measurements to be started immediately, rename the script named *startup* in your MS-DOAS project.

Whenever you want to stop all scripts and devices within MSDOAS, just click on the button with the crossed red circle on the top-left corner of the MS-DOAS window.

When first loading the *'Sky SerialNumber.mmp'* file, you need to adapt the following storage paths: Templog, Speclog, UV, Vis1. This can be done by left clicking on the respective device and then selecting



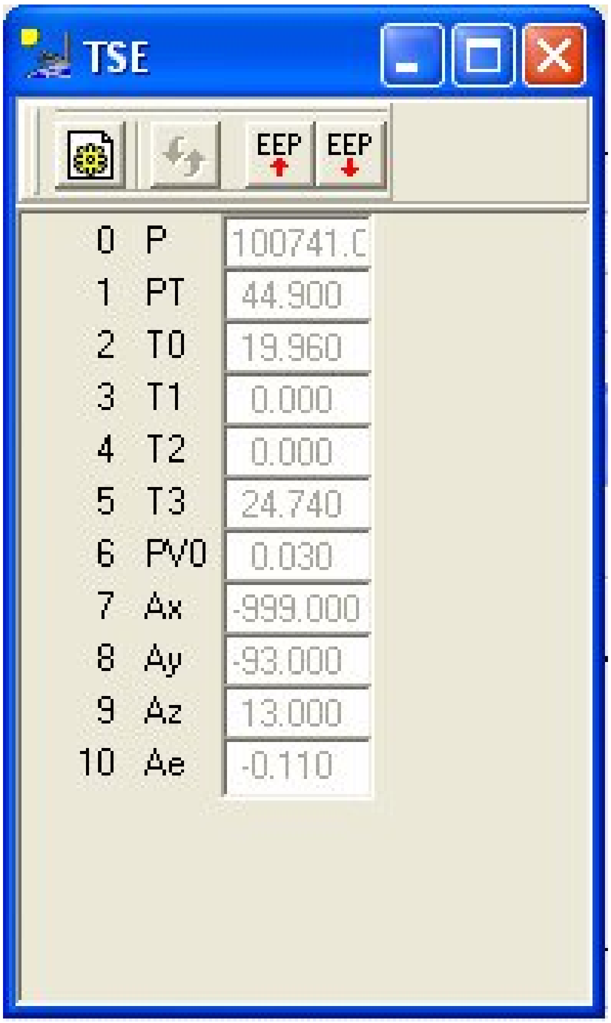
```
Auto - fixed tin  TExp: 82  TTot: 60000  Sat: 70
TAcq: 50351.5 Scans: 610   Max: 6983838 Min: 120266 Avg: 4074492 Name:   File:
SZA: 37.53 SAA: 186.12 LZA: 139.68 LAA: 19.99 LPH: 94.8% 21.08.13 11:43:23

Auto - fixed tin  TExp: 54  TTot: 60000  Sat: 70
TAcq: 47980.2 Scans: 892   Max: 10208998 Min: 566914 Avg: 474089 Name:   File:
SZA: 37.53 SAA: 186.12 LZA: 139.68 LAA: 19.99 LPH: 94.8% 21.08.13 11:43:23

21.08.2013 11:36:07 AM  Connection to Avantes Spectrometer 1212142U1 established.
21.08.2013 11:36:11 AM  Connection to Arduino established.
21.08.2013 11:36:13 AM  Connection to Arduino Stepper  established.
21.08.2013 11:36:25 AM  "Starting Measurement in 30 Seconds..."

SZA: 37.89 SAA: 191.86 LZA: 138.79 LAA: 24.98 LPH: 94.9% LAT: 49.50 LON: 8.66      21.08.2013 11:58:16 A
```

Figure 4.1: MS-DOAS Overview: Spectrometer windows have been opened and show spectra representative for zenith sky straylight measurements. In the UV window the channel number on the x-axis can be used to calculate the wavelengths. The part on the left in the far UV should contain almost no signal, since most radiation from the sun is absorbed by the ozone layer. Around channel 1200 two significant fraunhofer lines can be seen, caused by calcium absorption at the sun. The visible spectrum is not as structured, but also contains characteristic fraunhofer lines. Your spectra during daylight should look similar if the instrument is running fine. 1: Stop all scripts, 2: Properties of the spectrometer, 3: Single scan, 4: Continuous scanning, 5: Exposure mode, 6: Exposure Time, 7: Depending on Exposure mode: Total measurement time or number of scans.



0	P	100741.0
1	PT	44.900
2	T0	19.960
3	T1	0.000
4	T2	0.000
5	T3	24.740
6	PV0	0.030
7	Ax	-999.000
8	Ay	-93.000
9	Az	13.000
10	Ae	-0.110

Figure 4.2: List of measurement values provided by the TSE, also logged into the temperature log file (templog): ambient air pressure (P) in Pascal, Temperature of the electronics (PT) in degree celcius, (T0-T3) Temperature sensors, of which here the first one is the temperature stabilized spectrometer, T1 is the telescope unit, T2 are not connected and T3 is the outside temperature, (PV0) power with which the peltier element is driven for temperature stabilization and below acceleration values and the angle under which the telescope looks into the sky.

properties to change the path were the data will be stored. Furthermore the *COM port* onto which the controller electronics is connected needs to be selected from the property window of the *TSE* device. The port number can be obtained from looking into the device manager of Windows, there it will be found in the folder *Serial Connections* and the device is called *USB-to-Serial Adapter* Figure 4.3. After these changes, the project file can be saved and is ready to be used next time. To start measurements, select the *Measurement* device and press *play*.

If you do not have a NMEA-capable GPS mouse attached to your computer and added it as a device to MS-DOAS, then you need to manually enter your geoposition in MSDOAS. You can do this by double-clicking on the status bar and entering the correct values for latitude and longitude.

More than one spectrometer box

If you have more than one spectrometer box, connect the telescope scanner unit to one of the spectrometer boxes (which one might be indicated on the front of the box) and connect only this box to the computer. Check the COM port the TSE device is using and set it to the correct port if necessary as explained above. Then connect the other spectrometer box and set the COM port of the TSE2 device in MS-DOAS to the port number indicated in the device manager.

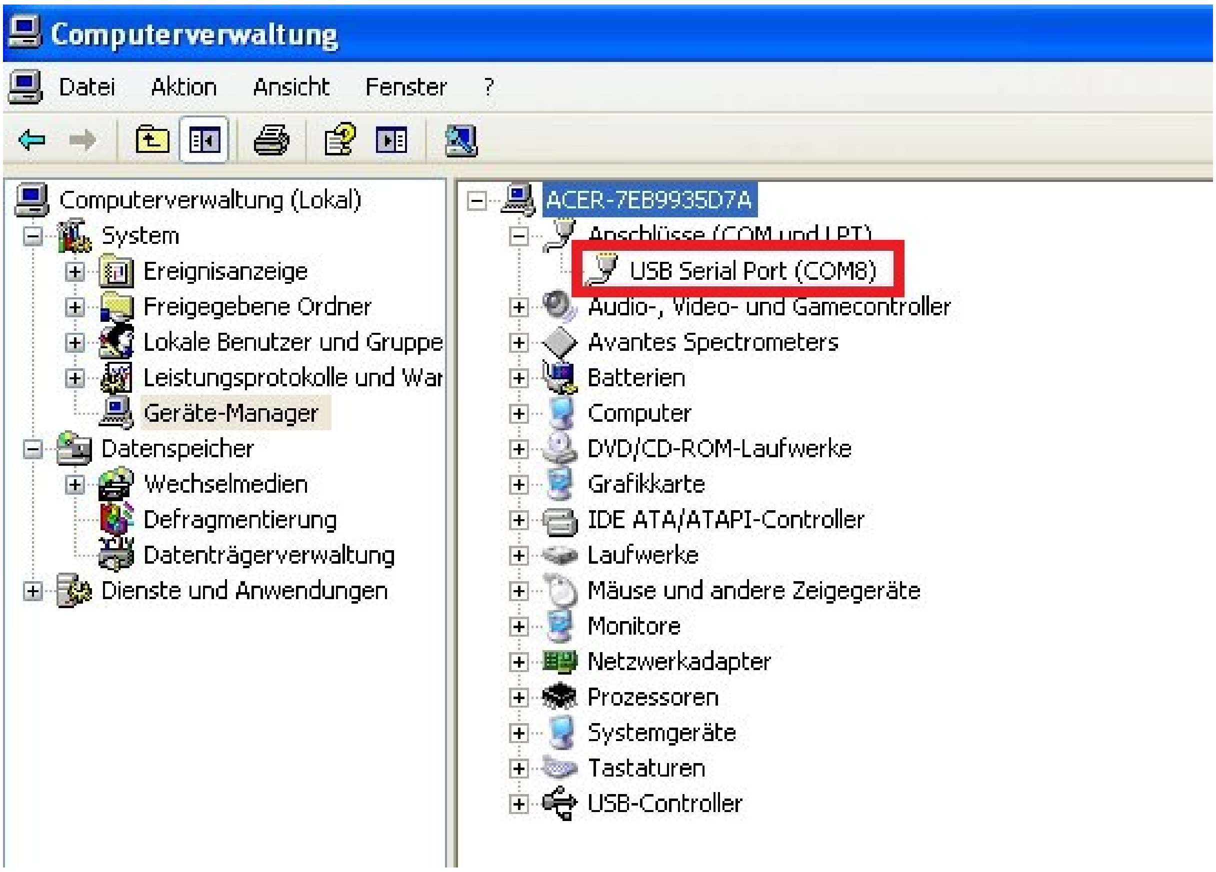


Figure 4.3: System Control Panel - Hardware Mananger of Windows : Here the COM-port number can found which has to be entered in MS-DOAS to connect to the temperature controller.

For each instrument there might be an additional configuration file called *'Sky SerialNumber.mmp'* which already contains the correct serial number in the property window of each of the spectrometers. If such a config file has not been delivered or the spectrometers have not been found, click on the properties button within the spectrometer device window and change the serial number of the spectrometer accordingly. A list of available serial numbers will be shown, the serial number of the spectrometers used in your Airyx SkySpec instrument can be found in the instrument test protocol.

4.1.2 The measurement script

The default measurement project for MS-DOAS also contains a measurement script for MAX-DOAS measurements, called 'Measurement' in the left menu among other 'devices'. Most of its variables are defined at the top of the script and are commented to explain their function.

```
;
; Measurement Script  MAX-DOAS
; Udo Frieß
;
; Version 20130821TSE Airyx GmbH
;
;



; Measurement Parameter

MaxSZA = 97      ; Max. SZA for scattered light measurement
MaxOffAxisSZA = 85 ; Max SZA for off-axis measurements

; Calibration spectra measurements
; Note: both calibration measurement criteria can be combined!
CalibBySZA = 1  ; Set to one (or zero if not) if the decision for the calibration measurements
                ; should be done based on SZA. This might not be always useful in polar regions
CalibSZA = 110  ; Min. SZA for calibration measurements

CalibByTime = 1 ; set to one if you want the calibration measurements done in certain fixed
                ; time intervals, such as once per week.
CalibTimeInterval = 7 + 1/24  ; define the interval in days in which calibration measurements
                              ; should be done. note that adding something like 1/24 will
; shift the calibration by one hour per calibration, which avoids
; regular measurement gaps at a certain time of day
CalibTimeLast = 0   ; Last time calibration spectra were recorded

; ExcludeAngle=0 disables checks
ExcludeAngle = 0 ; angle at which close to the sun no measurements should take place
ExcludeViewingDirection = 300; viewing direction of telescope (0 is north, 90 east, 180 south)

; ElevMode
; 1: each elevation angle and their respective scan number needs to be specified
; 2: Min, Max Elevation are given, with stepsize
ElevMode = 2;

; definitions for ElevMode = 1;
n_Elev = 17 ; Number of ElevMotor angles
ElevDir = 1 ; direction of elevation angles. 1 is "normal"
ElevOffset = 0; ; is there an offset?
Elev = 90, 40, 20, 10, 7, 5, 3,2,1,140,160,170,173,175,177,178,179    ; ElevMotor angle sequence
```

```
texp_uv_default = 500,500,500,500,500,500,500,500,500,500,500,500,500,500,500,500,500,500;
// default exposure times, will be changed while program is running
texp_uv = texp_uv_default;


; definitions for ElevMode = 2;
ElevMin = 10
ElevMax = 170
ElevStep = 10


; insert here latitude and longitude. This information is crucial to calculate the correct sun pos
lat = 49.5
lon = 8.66

; Aquisition Mode:
; 1:   Total integration time per elevation angle is fixed, exposure time is adjusted according to
; 2:   Total scan number per elevation time is fixed, exposure time is adjusted according to satur
SpecAquMode = 2

; The desired saturation of the spectrum
SpecSaturation = 50;

; for SpecAquMode = 1
; Time per elevation angle for a SZA lower than 80, 90, 92 degrees
; and a default value (in milliseconds)
TimePerElev80 =  6000
TimePerElev90 =  9000
TimePerElev92 = 12000
TimePerElev   = 30000

; for SpecAquMode = 2
; Number of scans per Elevation angle
ScansPerElev = 100


; due to a bug in the SZA routine of MSDOAS, sometimes calibration measurements are done during th
; as a bugfix, you can specify whenever there should be no calibration measurements,
; e.g. in Europe between 10-14 UTC
nocalib_start = 10
nocalib_end = 14

; settings for atuomatic calibration measurements
time_per_calib_spec = 60000
texp_dc = 10000
texp_ofs = 10
texp_hg_uv = 300
texp_hg334_uv = 5000
number_of_spec = 3;


;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
```

```
; from here on the code does not need to be changed in
; normal operation mode, except if bugs need to be fixed.
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
```

4.1.3 The measurement script - 2D sun tracking modes

These variables control the direct sun measurements. The idea behind the routine 'measure_directsun' is to look for the sun at its expected location, do some finetuning of azimuthal and elevation offset and then track the sun during the exposure of the direct sun spectrum according to calculated SAA and SZA, if the minimum intensity of 'directsun_minintensity' is reached. The finetuning of azimuthal and elevation offset is necessary, as the diffuser plates can create some small offset from the expected values.

'azi_offsetdegree_default' is the default offset of the instrument and should be determined in a best way possible, in order to keep the search area defined by 'azi_offsetdegree_search' small and thus to avoid too much time without measurements.

```
; define the intensity (counts per 3ms) at which the direct sun measurement should be stopped
directsun_minintensity = 4000

; Azimuth motor settings
azi_offsetdegree_default = -102;          offset of azimuth for the current setup
azi_offsetdegree = azi_offsetdegree_default;
azi_offsetdegree_known = 0;       >0 if we know the offset already to +-2°
azi_offsetdegree_search = 50;  how large should the interval be in which the sun will be searched. Use
azi_search_known = 1;        search sun within +-azi_search_known when azimuth offset is already known

; this is the offset as determined here from the routine in the last run
azi_SAAoffset = 0;
elev_SZAoffset = 0;

; check direct sun every 3 minutes; if this is smaller than 1 second, no scattered light measurement ar
checkdirectsun = (3.0/60.0)/24.0;
; checkdirectsun  = 0; uncomment if only direct sun measurements are wanted
; if no sun is found, add this wait time additionally (the brackets are needed as MSDOAS does not reall
checkdirectsun_addtime = (0/60)/24;

; how many spectra maximally:
max_spec_directsun = 5;
```

4.1.4 Temperature settings

In MS-DOAS the settings of the temperature controller can be found in the TSE device, called **'Cooling'**: The following variables can be modified. Do not change these values unless you know exactly what you are doing. Otherwise you might not be able to obtain stable measurements from your instrument.

- **Temperature** - not used
- **SetPoint** - the temperature that should be used for both spectrometer (default: 20)
- **P** - P parameter of the PID controller (default: 0.50) [1]
- **I** - I parameter of the PID controller (default: 0.05)

---

[1] Some devices need PID settings as (0.7; 0.03; 1)

- **D** - D parameter of the PID controller (default: 1.00)
- **Scale** - Scale parameter: scales PID controller output. Can be used to compensate for a Peltier connected in the wrong direction. (default: 1)
- **Mode** - Mode of the temperature controll: -1: cooling only, 0: normal, +1: heating only. (default: 0)
- **Max. PWM** - Maximum power of temperature controll. 0 is minimum, 255 the maximum value allowed. (default: 255)
- **PWM** - not used

The output of the temperature regulation electronics TSE can be seen in the main TSE window:

- **P** - ambient pressure
- **PT** - Temperature close to the temperature control electronics board
- **T0** - spectrometer temperature
- **T1** - normally not used
- **T2** - normally not used
- **T3** - outside temperature at telescope scanner box
- **PV0** - Cooling/Heating current of spectrometer temperature regulation, maximum values are -1 and 1.
- **Ae** - Elevation angle
- **Ax,Ay,Az** - raw acceleration sensor output
- **TA** - acceleration sensor temperature

The newer electronics (MCU) provides further variables, which can useful to monitor the instrument:

- **TSAM** - Temperature of the controller
- **TP** - Temperature of pressure sensor
- **HP** - (rel.) Humidity at pressure sensor
- **HC** - Current [A] to internal USB devices
- **T0s-T3s** - Standard deviation of the temperature sensors within one second. Typically values above 0.1 indicate potential malfunction
- **P,I,D** - Contribution of each part of the PID control
- **Aes** - Standard deviation of measured elevation angle

4.1.5 Adding a GPS device in MSDOAS

First install the driver of the GPS device. To add a GPS mouse to the MS-DOAS project, add a new device via 'New/Tracking Device/GPS Receiver'. The receiver needs to support NMEA output via a serial interface, which is the case for most typically used GPS mice. Use the properties to select details and set the system clock, if necessary. Longitude and Latitude in the spectra will be updated automatically.

4.2 DOASIS - Evaluation Software

DOASIS ([Kraus, 2006]) has been developed by the University of Heidelberg and Hoffmann Messtechnik and can be used via the graphical user interface or by using Java script code to automate work-processes. It comes already with an in-depth user guide and an extensive amount of documentation, therefore this instrument description is limited to the most important features of DOASIS. DOASIS is based on the Microsoft(R) .net environment and can be scripted using JScript programs.

Note that the DOASIS license is for non-commercial use only.

Within the *Help*-menu, the most important introductions to DOASIS, JScript and the internal functions of DOASIS can be found:

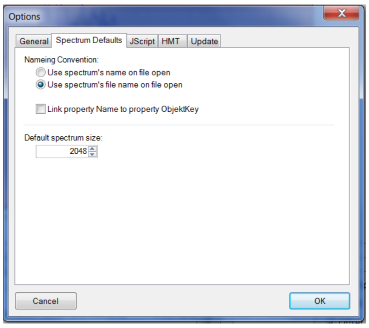
- DOASIS overview: To get to know basic information about DOASIS, system requirements and Version information
- DOASIS tutorial: get started with DOASIS
- JScript tutorial: If you are now familiar with JScript and you want to use DOAS data evaluation scripts using DOASIS written in JScript, this is the tutorial which can give you a fast and easy introduction to scripting. Simple examples and basic information about JScript is provided.
- Programming documentation: Once you are familiar with JScript, you have the possibility to access almost any internal DOASIS function. Each of them is documented in the Programming documentation, as well as necessary data types. This source of in-depth information requires a certain minimum of JScript knowledge, but can also easily be understood with previous knowledge of any object-orientated programming language of your choice, such as e.g. C++, C# or Java.
- Microsoft JScript online: Collection of information about JScript on the web.

As always, basic JScript problems and their solutions can often be found by using an internet search engine. If problems in one of your scripts appear, it is advisable to address them one-by-one, starting with the first one. This excludes the possibility that you first solve any follow-up errors based on a previous error or typo in your script.

4.2.1 Evaluation Script

An evaluation script for the analysis of MAX-DOAS data is available for DOASIS. Since it is based on DOASIS, the same restrictions on its usage apply as for the main program.

Before starting any script, open DOASIS, go to 'Extras/Options/Spectrum default/' and select 'Use spectrum's file name on file open' and disable 'Link property Name to property Object key', then click on OK. Furthermore, create a new spectrum with arbitrary name ('File/New') and 2048 channel.



Nameing Convention:
○ Use spectrum's name on file open
● Use spectrum's file name on file open

☐ Link property Name to property ObjektKey

Default spectrum size:
2048

Figure 4.4: Required changes to the options of DOASIS.

Whenever you installed the evaluation script new on a computer, you need to change directory paths accordingly in the following files: *eval01lp conv.jsp, eval01lp conv.js, eval01lp conv uv.jsp, eval01lp conv uv.js* and eventually *doasconsole eval.bat.*

The main configuration file is called *eval01lp conv.js.* Here all important variables and settings can be changed. This evaluation script needs an offset and dark current corrected and wavelength-calibrated mercury discharge spectrum, raw offset and dark current spectra[2]. The measurement spectra will be loaded from a path to be defined within the configuration script. The script comes with a collection of literature cross sections[3].

The script contains a mode which allows for the continuous analysis of spectra, it waits for several minutes whenever no further data is found. If there is already an output folder, the script will start again where it stopped last time. To start your script, start the corresponding *.jsp* file in DOASIS (docking window 'script' (bottom of the screen), start) or if you want to run it faster, start the corresponding batch file *doasconsole eval.bat.* This will then start the script in the DOASIS console, which typically runs faster, since the GUI does not need to be updated.

The script also contains basic functionality to run an analysis like proposed in [Vogel et al., 2013] to enable the user to evaluate the DOAS retrieval interval dependency of his results for each elevation sequence.

```
// define your paths on your local drive
var sBasePath = "C:\\";
var sCampaign = "compactMAXDOAS"

// should the I0 effect be corrected?
var bCorrectI0 = true;
// should a lowpass filter be applied to measured spectra and convoluted XS?
var g_iLowpass = 0;
// wait for new spectra once we are at the end of the spectra?
var g_iWaitfornewSpectra = 1;

// define paths in detail:
// where to find the spectra
var sPath = "c:\\spectra\\";
// where can calibration files be found?
var sCalibPath = sBasePath + "\\" + sCampaign + "\\";
// Where to store the evaluation results?
var sEvalPath = sBasePath + "\\" + sCampaign + "\\eval\\evaluation001\\";
// Where are the literature cross-sections?
var sLitSpectraPath = "d:\\evalscript\\Literaturspektren\\";

// Names of calibration files for the spectrometer.
// Raw Offset and DarkCurrent files. Do not ofs-correct DC or vice versa!
var sOffsetFile = "ofs.sp2";
var sDCFile = "dc.sp2";
// The HG discharge spectrum needs to incldue the pixel/wavelength calibration
// of the instrument included as a polynomial
var sHGFile =  "Hg.sp2";

// for the case of Fraunhofer calibration, where to find it.
var sfraunhofercalibrPath = sCalibPath;
var sFraunhoferCalibFS = "fraunhofercalibr.fs";
```

---

[2] 'raw' means here: without having applied any corrections

[3] We do not guarantee for the correctness of the spectra provided. For a detailed analysis, please check all used cross sections and the respective literature.

```
var sFitScenarioPath = sCalibPath;

// Should the measurement spectra be preshifted according to Fraunhofer
// Calibration? If the spectrometer is stable, this is typically not needed
var bShiftMeasFraunhoferfit = false; // should be correct the actual measurement spectrum?
var fShiftMeasFraunhoferfit = 0; // and if yes. by what amount?

// Are the spectrum files stored with the wrong order of channels?
// typically not.
var  bFlipSpectrum = false;


// Where to start the spectral evaluation, where to stop
var iFirstSpectrum = 1;
var iLastSpectrum  = 3000000;

// do Retrieval-Interval Mapping. For details: Vogel et al 2013
var gMAP = false; // do maps?
var gMAP_RMS = 1e-3; // max rms for map
var gMAP_Name = " 2"; // maps for this name
var gMAP_lower = 300; // lower bound
var gMAP_upper = 1100; // upper bound
var gMAP_min = 80; // min width
var gMAP_max = 6000; // max width
var gMAP_stepsize = 5; // stepsize in channel


// Which HG Peak to be used for convolution?
var HGConvLow  = 360; // 334nm peak
var HGConvHigh = 470;

// Should the minimum or a predefined value be substracted from the
// peak in the given HG file?
var substractMinimum = false;
var substractMinimumDefault = 241611.79700000002;

// If evaluating against a fixed noon spectra, decide on which to use
var iFixedNoonSpectrum = 4629;

// If evaluating against a summed fixed noon spectra, decide on which to use
var iFixedNoonSpectrumStart = 990;
var iFixedNoonSpectrumEnd = 1010;

var bSuspendEvents = 0;

// When using automatic references, which spectra name is typically to be used
// as a reference?
var refName = "90";
var iMinRefScans = 0; // Min number of scans to use spectrum (quality assurance)

var o4peak = 360.8;
var IntensityAverage = 1161;
```

```
var IntensityAverageWidth = 6;


// define how spectra had been stored
var MeasFile : AutoFileName = new AutoFileName();
    MeasFile.BasePath = sPath;
    MeasFile.Prefix = "U";
    MeasFile.Mode = 1;
    MeasFile.Suffix = "";
    MeasFile.NumberOfDigits = 7;
    MeasFile.FilesPerFolder = 100;
    MeasFile.CurrentFileNumber = iFirstSpectrum;


[....]

// co-adding spectra
// If you want to co-add spectra with the same name, you can enable this here
var g_bSum = false;
var g_iNumSum = 4; // anzahl summierungen
var g_iMaxDiff = 9*(g_iNumSum+1);
var bSaveSummedSpectra = true;

[....]

// summieren ende


// define which spectra should not be evaluated as normal DOAS measurements
var psNightName : Array = new Array;
psNightName[0] = "Offset";
[....]

//  fraunhofer reference spectrum calibration
var pFitFraunhofer = [false,false,false,false,false,false];
var pFitFraunhoferDefault = [true,true,true,true,true,true,true,];
var pFitFShift = [0,0,0,0,0,0,];
var pFitFSqueeze = [0,0,0,0,0,0];
var pFitXSIndex = [2,2,2,2,2,2];

var bWeHaveAlreadyDC = 1; // we have already DC and Offset
var bSaveResiduum = 1;    // should we save our residuums
var bSaveReference = 0;    // should we save our residuums
var bSaveFitScenarios = 1;    // should we save our FitScenarios
var bSaveCMeasSpec = 1;    // should spectra be saved which are actually fitted?

var bFixedReference = false;    // fixed reference in fit scenario ?
var bFixedReferenceSummed = false;    // summed up fixed reference ?
var bCurrentReference = true ;   // if no fixed reference. use Current Reference ?
var bCurrentReference1 = false;
var bNoonReference = false;   // if no fixed reference. use Noon Reference (min SZA during the day
```

```
// define here which solar reference spectrum you would like to use
SKuruszRaw.Open(sLitSpectraPath+'irradthuwl_air.sp2');

// which wavelength should be used to 'orthogonalize' the RingSpectrum4 spectrum against?
var g_Ring4Middle = 340;

// fit scenarios
var pFitScenarios = ["bro.fs","so2.fs","o4.fs"];
var pFitNames = ["BrO","SO2","O4"];

// to transfer fit coefficients from one fit szenario to another:
var pCopyFrom =  []; // from which fit szenario
var pCopyTo   =  []; // to which fit szenario
var pCopyWhat =  []; // and which XS, e.g. 'H2O'


var pFitRMSIgnore = [1000,1000,1000,1000,1000,1000];//above which rms the fit should be ignored

// define here the cross-sectionsto be used, their default shift and the respective XS file
var pGasNames = ["BrO","HONO","NO2_220K","NO2_294K",[....]];
var pGasShift = [...];
// thalman
var pGasLFiles = [...]
```

When you look for detailed information about certain variables, the easiest way to obtain these is to look in the main.js and func.js files for the respective variables.

4.2.2 Choice of Fraunhofer reference spectra

If the main purpose of the measurements are retrieval of homogeneously distributed tropospheric absorbers, choosing the nearest or an arbitrary zenith sky spectrum (90°) as Fraunhofer Reference spectrum (FRS) is reasonable to avoid the influence of stratospheric absorbers and minimize measurement errors. Furthermore this minimizes the danger of being influenced by instrumental instabilities. At volcanoes or local emission sources, it might make sense to select a suitable and fixed, 'absorber free' spectrum as a reference, since here also zenith sky spectra can be 'contaminated' by absorptions of the trace gas of interest. To get an overview over measurements under such conditions, also a noon reference can be useful. All of these alternatives can be selected from the evaluation script by setting one of the reference spectrum options to *true*:

```
var bFixedReference = false; // fixed reference in fit scenario ?
var bFixedReferenceSummed = false; // summed up fixed reference ?
var bCurrentReference = true;  // if no fixed reference, use Current Reference ?
var bCurrentReference1 = false; // only one reference spectrum, otherwise two nearest spectra
var bNoonReference = false; // if no fixed reference, use noon Reference ?
 // (index set in iFixedNoonSpectrum)
var bNoonReferenceTime = false; // use a fixed noon reference at fNoonReferenceTime?
var fNoonReferenceTime  = 11.5;  // time of fixed noon reference when selected
```

4.2.3 Fit scenarios: Literature absorption cross-sections and built-in spectra

The fit scenario files (*.fs) define the DOAS fit as it is executed from within the evaluation script. These can be loaded explicitly into the DOASIS GUI in order to manually inspect the fit itself (see section 4.2.5). The fit scenario file defines the polynomial used, the additional (intensity) polynomial and the cross-sections and spectra fitted to the measurement. The literature cross-sections are not directly added into the fit scenario, but instead, spectra with one of the names listed in 'pGasNames' in the config file can be added to the fit scenario. When running the script, these placeholders will be replaced by a spectrum, which is calculated by convolution from the literature cross-section files listed in 'pGasLFiles' applying saturation and I_0 correction according to the numbers given in 'pI0Coeff' and being shifted by the entry defined in 'pGasShift' (in nm). Make sure that the spectra in the fit scenario are linked to each other, if necessary.

The evaluation script does not only replace the placeholder spectra in the fit scenarios for each of the absorbers, but also replaces a number of spectra listed below. The spectra are either calculated from the reference spectrum itself or from the convoluted literature cross-section files. [4]

	Name	**Description**	Possible citations:
1	ReferenceSpectrum		
2	RingSpectrum	calculated (T=273K, 20% O_2) from **1** according to	[Bussemer, 1993]
3	RingSpectrum4	Wavelength dependence of **2**	[Wagner et al., 2009]
4	RingSpectrumCold	Temperature dependence of **2**	
5	RingSpectrumVRSN2	VRS N_2 correction calculated from **1**	[Lampel et al., 2015a]
6	RingSpectrumVRSO2	VRS O_2 correction calculated from **1**	
5'	VRSN2	VRS N_2 correction (solar atlas)	[Chance and Kurucz, 2010]
6'	VRSO2	VRS O_2 correction (solar atlas)	
7	XS	convoluted cross section of absorber XS	
8	XS_dL	Wavelength dep. of AMF of absorber XS	[Puķīte et al., 2010]
9	XS_dSq2	Absorption dep. of AMF of absorber XS	[Puķīte et al., 2010]
10	XS_dSat	Linearization of saturation effect (Diff. between conv. XS at SCD_{I0} and at 0.9 SCD_{I0})	[Wenig et al., 2005]
11	XS_dI0	Linearization of I_0 effect	

Table 4.1: Built-in spectra, which get replaced in the evaluation JScript in the respective fit szenarios once when executing the script (7-11) or for each new reference spectrum (1-6).

4.2.4 Suggested evaluations

Some fit scenario files are included with the evaluation script (*.fs files). These are preconfigured for your instrument, but can easily be changed. Note that depending on your measurement site, abundance of different trace-gases and used measurement geometries the wavelength intervals for the evaluations of different species might vary and are still always a matter of discussion and also instrumental capabilities. For the evaluation of BrO different fit intervals are e.g. discussed in [Aliwell et al., 2002, Vogel et al., 2013] and references therein. For DOAS fits with RMS below 2×10^{-4} vibrational Raman scattering on air molecules might need to be considered [Lampel et al., 2015a] for wavelength ranges above 330 nm.

Broad wavelength intervals or intervals encompassing strong line-like absorption peaks need to consider changes of the AMF with wavelength and/or absorption itself, as e.g. suggested in [Puķīte et al., 2010].

For total column NO_2 and O_3 NDACC guidelines can be found on the NDACC website [5] [6]. These might however require updated cross-section files, especially for O_4 ([Thalman and Volkamer, 2013]) and H_2O ([Rothman et al., 2010]) absorption cross-sections.

---

[4] Note that for the NDSC Ring literature cross-section, you need to convolute and divide the corresponding spectra manually using the GUI in DOASIS and copy it to your fit scenario (not using the name 'RingSpectrum', as that would be replaced). This type of Ring spectrum is not yet supported in the evaluation script.

[5] `http://ndacc-uvvis-wg.aeronomie.be/tools/NDACC_UVVIS-WG_NO2settings_v4.pdf`

[6] `http://ndacc-uvvis-wg.aeronomie.be/tools/NDACC_UVVIS-WG_O3settings_v2.pdf`

	NO_2	SO_2	BrO	HCHO	O_4	IO	H_2O	Glyoxal	S_{I0}
Start [nm]	425	315	332	336	350	415	432	432	molec/cm^2
End [nm]	498	327	358	359	373	440	450	458	
Polynomial	4	3	3	3	3	3	3	3	
Add. Polynomial	1	1	1	1	1	1	1	1	
Ring	X	X	X	X	X	X	X	X	
Ring$\cdot\lambda^4$	X	X	X	X	X	X	X	X	
SO_2		X							
O_3 223K	X	X	X	X	X	X	X	X	$1 \cdot 10^{18}$
O_3 243K		X	X	X					$1 \cdot 10^{18}$
BrO		X	X	X	X				$3 \cdot 10^{13}$
HCHO		X	X	X	X				$5 \cdot 10^{15}$
HONO			(X)	(X)	(X)				$1 \cdot 10^{15}$
O_4	X		X	X	X		X	X	$3 \cdot 10^{43}*$
NO_2 224K			X	X	X	X			$5 \cdot 10^{15}$
NO_2 294K	X	X	X	X	X	X	X	X	$5 \cdot 10^{15}$
H_2O	X					X	X	X	$3 \cdot 10^{23}$
IO	(X)					X	X	X	$3 \cdot 10^{23}$
Glyoxal						(X)	(X)	X	$5 \cdot 10^{14}$
liq. H_2O	(X)						(X)	(X)	
liq. H_2O VRS	(X)					(X)		(X)	

Table 4.2: Suggestions for retrieval wavelength intervals for MAX-DOAS measurements (*) in molec^2 cm^{-5}. These settings are not binding and maybe also depend on instrument properties and covered wavelength range. Furthermore some of the species listed are not ubiquitous found in the troposphere, as e.g. halogen oxides, HONO and Glyoxal.

Ring	[Bussemer, 1993], DOASIS [Kraus, 2006]
Ring$\cdot\lambda^4$	[Wagner et al., 2009]
SO_2	[Bogumil et al., 2003] or [Vandaele et al., 2009]
O_3	[Serdyuchenko et al., 2014]
O_3	[Bogumil et al., 2003] (for SO_2)
BrO	[Fleischmann, 2004]
HCHO	[Chance and Orphal, 2011]
HONO	[Stutz et al., 2000]
OClO	[Kromminga et al., 2003]
O_4	[Hermans et al., 1999]
	[Greenblatt et al., 1990]
	[Thalman and Volkamer, 2013]
NO_2	[Vandaele et al., 1998]
H_2O	[Rothman et al., 2013] (HITEMP) with corrections [Lampel et al., 2015b]
	UV: see [Lampel et al., 2017]
IO	[Spietz et al., 2005]
Glyoxal	[Volkamer et al., 2005]
liq. H_2O	[Fry et al., 1992]
liq. H_2O VRS	[Dinter et al., 2015, Peters et al., 2014]

Table 4.3: Literature references for table 4.2.

4.2.5 How to inspect individual DOAS fits

The results of the fits are stored in the path given in *sEvalPath* variable. For each fitted quantity, a fit error is given.

Molecule	typ. Measurement error	SVMR error	typ. observed dSCD
SO_2	$7 \cdot 10^{15}$ molec cm^{-2}	300 ppt	below DL
O_3			(*)
BrO	$2 \cdot 10^{13}$ molec cm^{-2}	0.75 ppt	below DL
HCHO	$5 \cdot 10^{15}$ molec cm^{-2}	200 ppt	$(0-6) \cdot 10^{16}$ molec cm^{-2}
HONO	$5 \cdot 10^{14}$ molec cm^{-2}	20 ppt	$(0-6) \cdot 10^{15}$ molec cm^{-2}
O_4	$4 \cdot 10^{41}$ molec^2 cm^{-5}	-	$(0-4) \cdot 10^{43}$ molec^2 cm^{-5}
NO_2 (vis)	$7 \cdot 10^{14}$ molec cm^{-2}	30 ppt	$(0-4) \cdot 10^{17}$ molec cm^{-2}
H_2O	$1 \cdot 10^{22}$ molec cm^{-2}	0.5 ‰	$(0-6) \cdot 10^{23}$ molec cm^{-2}
HONO	$4 \cdot 10^{14}$ molec cm^{-2}	15 ppt	$(0-5) \cdot 10^{15}$ molec cm^{-2}
IO	$6 \cdot 10^{12}$ molec cm^{-2}	0.25 ppt	below DL
Glyoxal	$6 \cdot 10^{14}$ molec cm^{-2}	25 ppt	$(0-5) \cdot 10^{15}$ molec cm^{-2}

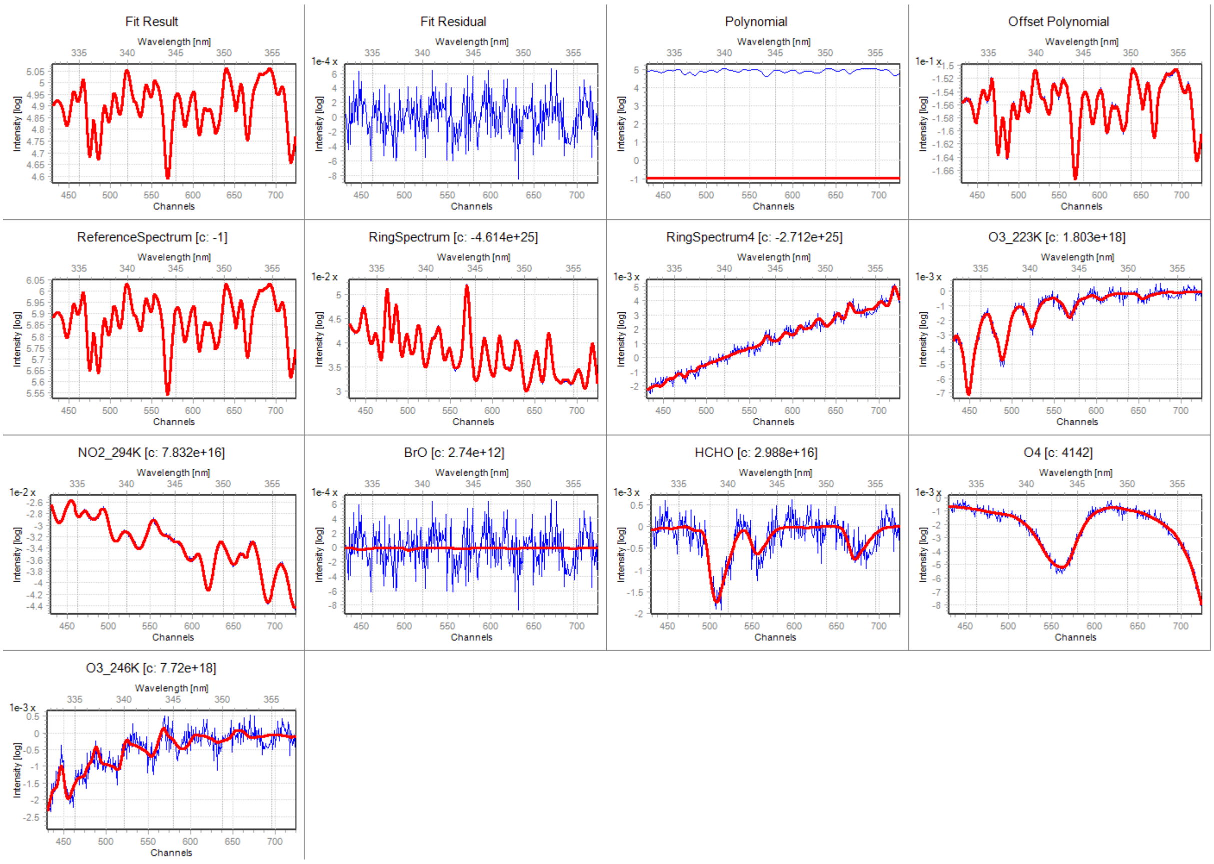
Table 4.4: Typical measurement errors (here: 2x fit error) and observed column densities during the MADCAT campaign in Mainz/Germany, 2013. Spectra were recorded for 60 s each. The 2x fit error estimate can be conservative in most cases. The second column is an estimate of the measurement error converted to volume mixing ratio (VMR) for a constant profile within the lowermost kilometre of the troposphere at a visibility of 10 km. Uncertainties and errors from aerosol and trace-gas profile retrievals can contribute significantly to the overall measurement error of the retrieved surface volume mixing ratios (SVMR). Co-adding measurement spectra typically reduces the measurement errors further, until uncertainties of literature cross-sections and insufficiently modelled radiative transfer effects limit the measurement accuracy. This reduces the effective time-resolution of the measurements. It strongly depends on the fit settings and the abundance of trace-gases, which could interfere. (*) retrieval of tropospheric concentrations typically not possible.

Often it is not sufficient to simply look at the DOAS fit results and their respective errors to estimate the significance of a result. First of all, the fit error often underestimates the measurement error by a factor of two, as it has been discussed e.g. in [Stutz and Platt, 1996]. Secondly, other absorbers can, if not taken into account correctly or left out, result in false results. If such a case is present, can often be judged from a detailed plot of a DOAS fit, showing all absorbers and also showing if the residual still contains systematic structures.

To take a look at such a fit, open the result file (e.g. *NO2vis all.txt*) and a select a line which seems interesting to you. In the column 'filename' you find the name of the spectrum. Look into your evaluation folder (defined in *sEvalPath*) to the subfolder *MeasSpec* and open the spectrum with the same running number in DOASIS. This spectrum is already corrected for dark-current and offset. Then open from your same evaluation folder the subfolder *fitscenarios* in which you find the fit scenarios including the convoluted cross-sections. Open a fit scenario in the fit window of DOASIS. If you cannot find this window, use 'View/Docking windows/Fitting' to get there. When you have selected your measurement spectrum from the Specbar, you can simply press '!' and the DOAS fit will be performed. In Figure 4.5 an example for the evaluation of BrO is shown.

4.3 Wavelength calibration

The pixel-to-wavelength mapping of your instrument is, as is the instrument line function, cruical for correct spectral retrievals. This wavelength calibration can either be obtained from a mercury discharge spectrum and the calibration assistant of DOASIS (Data/Calibration Assistant) or by using the calibration script provided in the subfolder *CalibrationSunlight* of your evaluation script. The exact procedure requires also a precalibrated mercury discharge spectrum and determines then the wavelength calibration by comparison of a solar atlas and a measured sun spectrum. More details can be found in *CalibrationSunlight/kurucz6 uv.js*.



Fit Result

Fit Residual

Polynomial

Offset Polynomial

ReferenceSpectrum [c: -1]

RingSpectrum [c: -4.614e+25]

RingSpectrum4 [c: -2.712e+25]

O3_223K [c: 1.803e+18]

NO2_294K [c: 7.832e+16]

BrO [c: 2.74e+12]

HCHO [c: 2.988e+16]

O4 [c: 4142]

O3_246K [c: 7.72e+18]

Figure 4.5: Example DOAS fit using an Airyx SkySpec (MAX-DOAS) instrument. The blue lines show the measured optical densities, while the red line shows the modelled optical densities according to the literature cross-section of each absorber. O_4 and Formaldehyde (HCHO) can clearly be identified, while BrO stayed below detection limit. (Note that this spectrum had an exposure time of 8 minutes, if you have an exposure time of 1 minute, the residual will be typically $\sqrt{8}$-times larger.)

Chapter 5

Practical Issues

5.1 Recording calibration spectra

NOTE: If you have an instrument with incorporated Hg-lamp and shutter, you can also record these spectra manually without having to disconnect the optical fibre from the scanner unit.

Before connecting the fibre to the scanner unit, it is advisable to record a new set of calibration spectra to be used within your spectral retrieval later on, to avoid an eventual influence of the transport of your device on the properties of the highly sensitive spectrometers. Three types of spectra are usually needed to characterize the basic properties of the spectrometer: a dark current spectrum, an offset spectrum and a spectrum of a HG calibration lamp. Once the instrument is continuously operated these spectra should be stable and a repetition of this procedure might only needed once per year. Dark current and offset spectra are recorded for all versions of the instrument at night time whenever the sun is sufficiently below the horizon ($SZA > 110$).

1. **Dark current spectrum:** Used to compensate for the dark current of the detector, a temperature-dependent effect caused by the properties of the semiconductor. The dark current is linear with respect to time (at least for practical purposes, for details see e.g. **??**). Use a long exposure time and a sufficient number of scans to record this spectrum with the black cap on the end of the fibre (suggestion: 10 scans at 30s).
2. **Offset spectrum:** The ADC (Analog-Digital Converter) of the CCD electronics cannot convert negative voltages which might occur due to noise. To avoid creating a bias, to all data from the CCD a constant value for each pixel in each scan will be added. To compensate for this, the offset spectrum needs to be substracted accordingly. Record a spectrum with a high number of scans at a small exposure time with the black cap on the end of the fibre. (suggestion: 10000 scans at 3ms).
3. **Discharge (HG or Ne) lamp spectrum:** This spectrum is used to characterize the response of the spectrometer to single emission lines as well as to create a pixel-wavelength mapping to be used later on during data evaluation. Record a spectrum each for each of the emission lines you want to use in your data evaluation in such a way that the emission line of interest is as well-exposed as your usual sunlight spectra in that spectral region. Record a spectrum for about one minute with a maximum saturation of 70%. If you need weaker lines for your later evaluation (as e.g. the line at 334nm for evaluation of BrO, ozone and formaldehyde) also record a separate spectrum with a longer exposure time to have a comparable saturation of the weaker lines.

5.2 Elevation angles

Default elevation angles are 90,40,20,10,7,5,3,2,1 degrees. These can be modified within the *'measurement'* script in MS-DOAS (subsection 4.1.2). To edit this file you need to stop it first. Eventually also the

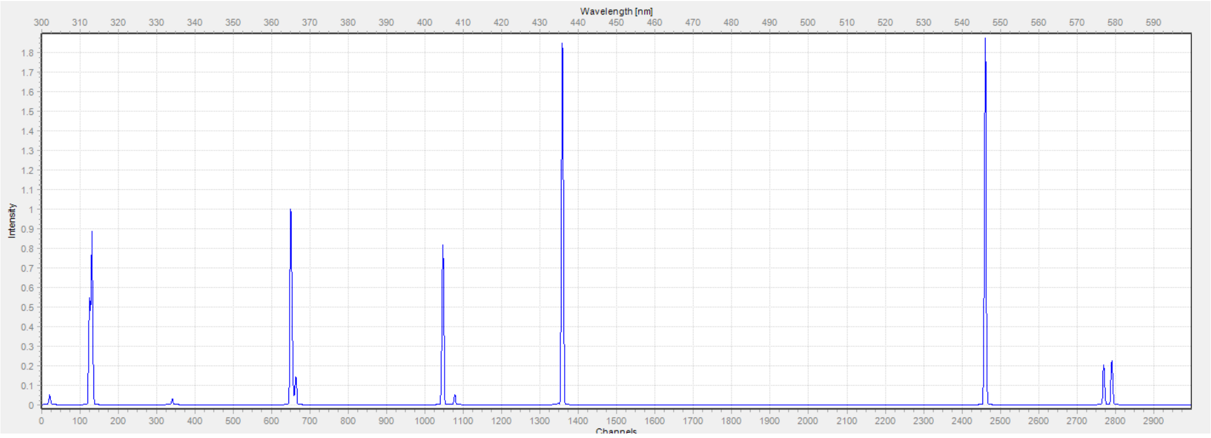


Figure 5.1: Hg emission lines from 300-600nm at a resolution of 0.5nm, adapted from [Sansonetti et al]. For spectral retrievals of measurement data only single lines can be used. In measured spectra a second order of the emission line at 253.7nm can be observed at 507.4nm, that line should not be used for evaluations.

number of elevation angles needs to be modified then.

The minimum elevation angle which can be used is -10° before the end switch is touched. Negative angles can be useful if the instrument is located high above the ground and appropriate radiative transfer can be done during evaluation.

When selecting elevation angles make sure that none of the viewing directions is obstructed by mountains, trees or a ceiling above the instrument. When no zenith viewing direction is available, an elevation angle close to 90° is usually sufficient for MAX-DOAS observations, such as 40 or 60°.

5.3 Calibration of the Azimuth angle

The determination of the azimuth angle depends on the installation of the instrument and needs to be determined manually. It is crucial to know it for inverting the dSCDs to obtain profile information. It can be determined by aiming at landmarks along the edge of the telescope unit.

[Sihler et al., 2016] presents a method to inversely determine the field of view using simultaneous image acquisition (with absolute intensity calibration, as e.g. from RAW data from a DSLR [1]). Also the field of view of a MAX-DOAS can be determined this way. Use of webcam or other jpeg-like image data however is typically not sufficient due to the unknown response curves of the respective camera and/or the image conversion before storage.

5.4 Temperature of the spectrometer

By default the set point of the temperature control of the spectrometers is set to 20°C, to avoid condensation within the instrument. It is not recommended to set a lower temperature as this will only insignificantly improve the measurement quality. It is rather recommended to set the temperature to a value close to the typical room temperature where the spectrometer is located. Lower temperature would reduce the dark current noise, but increase the danger of condensed water on the CCD chip, on optical filters and the spectrometer electronics itself. **This would degrade the instruments' performance significantly.**

---

[1] see also https://vimeo.com/162520417

For a ULS grade Avantes spectrometer which are often used in Airyx products, about 3% of the recorded spectrum are caused by the dark current (for a backthinned detector, less for regular CCDs). Since both photons and the electrons causing the dark current are governed by poisson statistics, the overall contribution to shot noise by the dark current is also small.

The temperature behaviour of the dark current follows a Boltzmann curve $\exp(-\frac{\Delta E}{k_b T})$. This results in a doubling of dark current for a temperature increase of about 5°C, but the noise dependens only via $\sqrt{n}$ on the dark current.

5.5 Power Supply

With the MAX-DOAS instrument a 110-220V power supply is included. For battery operated use or other types of power supply, use pin1 (10-16V) and pin2 (GND) of the power connector (HIRSCHMANN CA3GS). Please note that if the polarity of a power supply is wrong, the electronics might be damaged. In this case also the 10A fast fuse may melt. If the 10A fast fuse is melted, this will lead to a power disconnection. Please look then for the cause of the melted fuse before replacing it. It might be due to a damaged or wrongly connected power supply or an instrument malfunction. The fuse can be replaced from the outside.

The instrument uses maximally 100W for a short time when the temperature regulation is working at maximum power, constant power consumption at room temperature (15-30°C) was found to be below 20W. If the scanner is placed in a cold environment 0°C , additional heating power of 30W is required to heat the quartz cylinder to melt ice. (see also Figure 6)

Chapter 6

FAQ (Frequently Asked Questions)

Symptoms:

1. None of the spectrometer is responding in MSDOAS

   (a) USB connection ok?

   (b) Are the spectrometers listed in system's device manager? See Figure 3.1 and section 3.1. If not, reinstall them, restart the computer.

   (c) Are the spectrometers detected by AvaSpec? see section 3.2

   (d) Do the spectrometer have IDs in MSDOAS? like '1511019U1'? If not, you might have changed your USB port in between, or you had two programs (MSDOAS and Avaspec in parallel?) running which access the spectrometer. To fix this, close the other program if there was one, then go to the properties of the spectrometer window and select the according ID of the spectrometer. For systems with two spectrometers, make sure that you don't exchange UV and VIS spectrometer by accident. This can be easily seen by comparing previous spectra with current scattered sunlight spectra.

   (e) ...

2. The TSE temperature controller is not responding

   (a) USB connection ok?

   (b) COM port number correct? To check the COM port number, open the system's device manager as shown in Figure 4.3

   (c) Disconnect the USB connector and switch off power. Wait 1 minute, connect the USB plug again and switch on the power supply again. Check again.

   (d) Try to connect with a serial port monitor (RealTerm e.g.) to the COM port using 57600 baud. If no response at all appears, contact us.

   (e) Open the spectrometer box and see wether the USB hub is powered. If not, contact us.

3. The TSE device COM port has a number larger than 10. MS-DOAS only shows COM ports until 10. How can this be solved?
   Go to the properties of the COM port in *device manager* of windows. Go to advanced options. There the COM port number can be changed. You can mostly ignore the label "in use". This just mean there was a device before connected to the PC which was related to this COM port. You can just use one of them. Typically just COM1 and COM2 are really used by an other device, so if you

select e.g. COM6 it should work. You will directly see if there is a problem, as than the device will be labelled as "not working properly". Nothing can happen or be damaged if you just select such a COM port.

4. Is there a way to see if the TSE unit is properly working?
   Normally you should be able to the TSE unit with MSDOAS. Then you can see if it is working if whenever the data in the data output (main) window of the TSE (Figure 4.1) is changing. Another possibility is to connect to the serial port onto the specific COM port with a setting of 57600baud with a serial port monitor (RealTerm e.g.), and wait for a response. If you get a response, send 'log 4' with a carriage return and you'll be shown the data which is also shown normally within MS-DOAS.

5. How can I remove hot pixels from the auto-aquisition routine of MSDOAS?
   Open the property window of the respective spectrometer (top left icon in the spectrometer window) and select the auto-acquisition tab. There you can list individual pixels or ranges of pixel to be ignored when the auto acquisition mode determines the exposure time. Note that these pixels will still be stored in the final results and need to be explicitly considered in the spectral evaluation.

6. The spectrometer box was connected to a different USB port as before. Now all devices seem to be lost in MSDOAS - what to do?

   When the spectrometer box is connected to a different USB port of the notebook, the devices will be typically reinstalled, but can be found under a different name: E.g. the temperature stabilization unit (TSE) will get a new serial port number. This needs to be adapted in the property window of the TSE unit in MSDOAS. Also webcams and spectrometers might need to be reset to their actual device and serial number in order to work correctly. This can also be done from the respective property window of the device.

7. The webcams are not working, what to do?

   Make sure that the webcam is used in YUY2 mode and using a resolution of 720x480px (left side of webcam window in MSDOAS). Set the brightness and contrast controls to reasonable values in MSDOAS (typically in the middle of the slider), in case these have been changed. Do not use several webcam windows for one identical webcam, but use different devices instead. Use different webcam entries, even if they have the same name. If you try to access one webcam via different windows at the same time, this will lead to unreproducable errors or no response at all. If this does not help, use an external program (like yawcam) in order to set the properties of the webcam accordingly. For the video grabber based webcams, the mode needs to be set to 'PAL B', YUY2 mode and 720x480px. If a green bar is displayed at the bottom, the image resolution needs to be adjusted.

8. The measurement setup seems to crash always during the night - in the morning the computer does not recognize e.g. the spectrometers.

   Please check the Energy options of your computer: Individual ports and devices can use power saving modes if they are not used for a while. However, this can eventually lead to instabilities. Therefore we suggest to deactivate these power saving modes for the USB ports used for the MAX-DOAS devices. To do so, go to 'Device Manager', 'Universal serial bus controllers', 'Generic USB Hub', 'Properties' and 'Power Management'. Then deactivate the option 'Allow the computer to turn off these devices to save power'. Do this for all connected and relevant internal USB hubs.

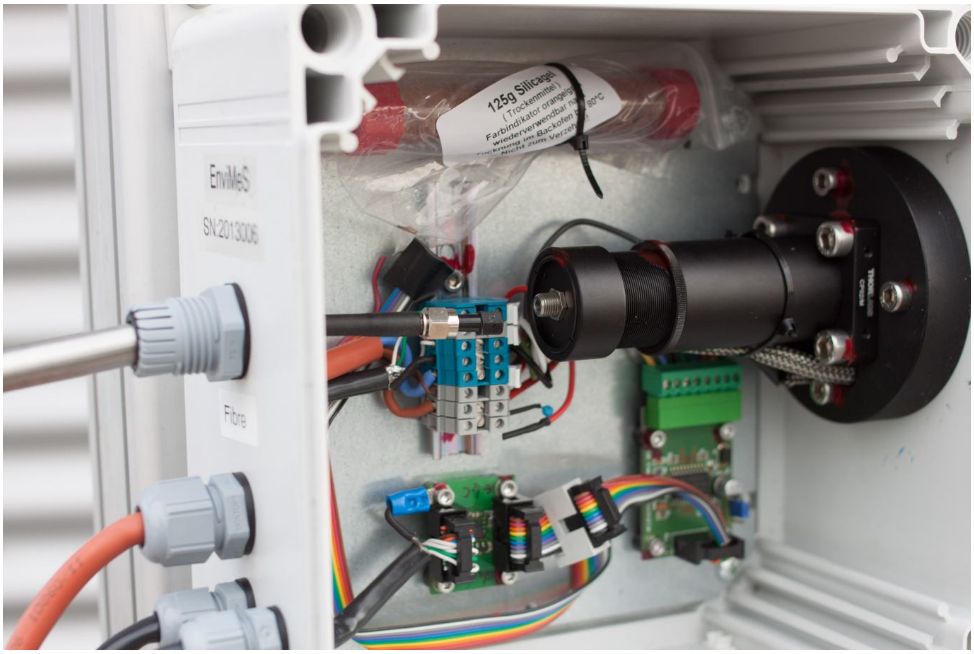


Figure 1: The PG plug on the left has been opened and the fibre has been moved into the scanner unit.

Figure 2: The end of the fibre, protected by a black cap. On the left the stainless steel tube can be seen which is used to close the scanner unit.

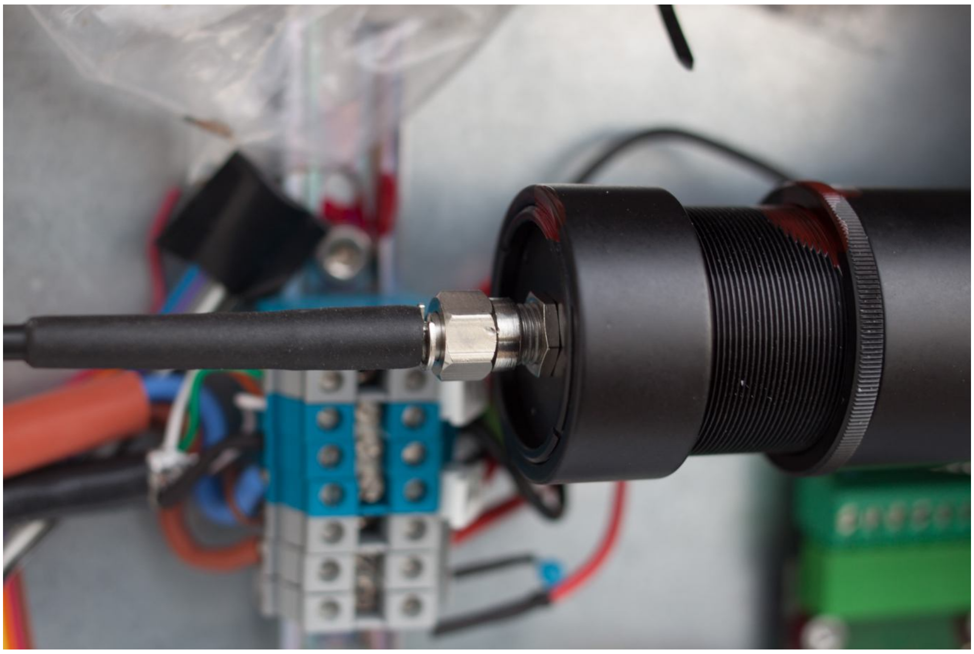


Figure 3: The fibre connected to the telescope tube via a SMA plug. The tube on the right has been carefully adjusted to obtain an optimal field of view. Do not turn!

Figure 4: Before tightening the PG plug, the fibre, the stainless steel tube and the rubber sealing should look like this.

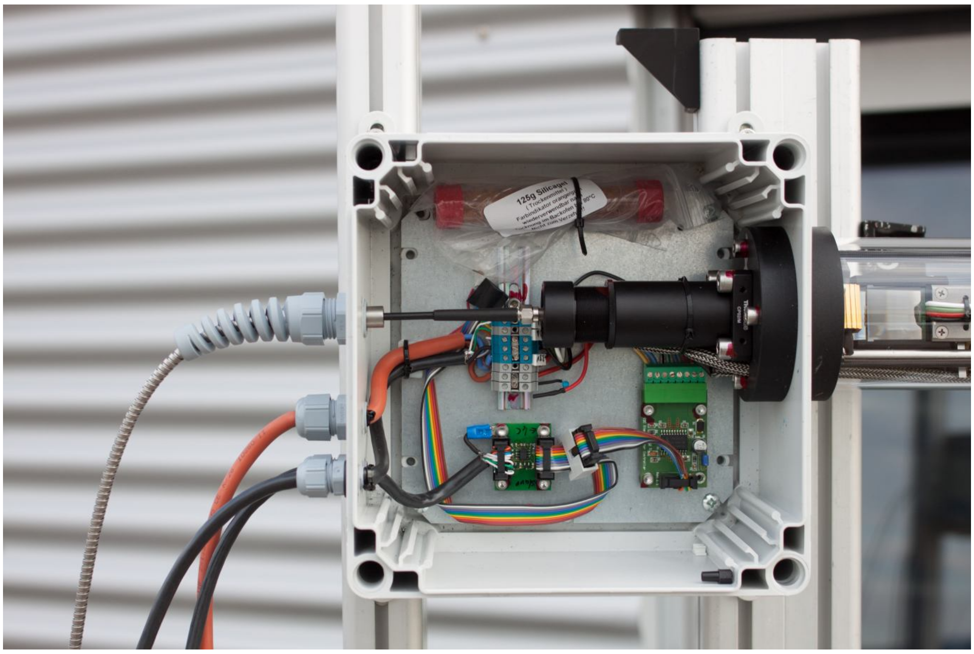


Figure 5: The Airyx SkySpec scanner telescope unit as it should look before opening the plastic bag with the desiccant and closing the lid.

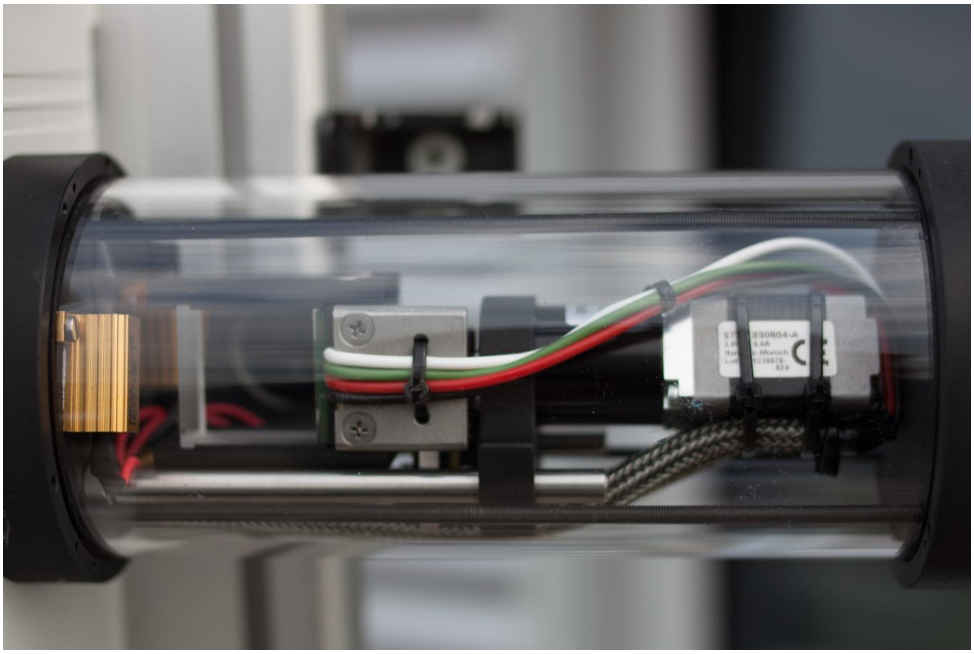


Figure 6: A detailed view on the quartz cylinder of the Airyx SkySpec telescope. On the left the heating resistors are visible.

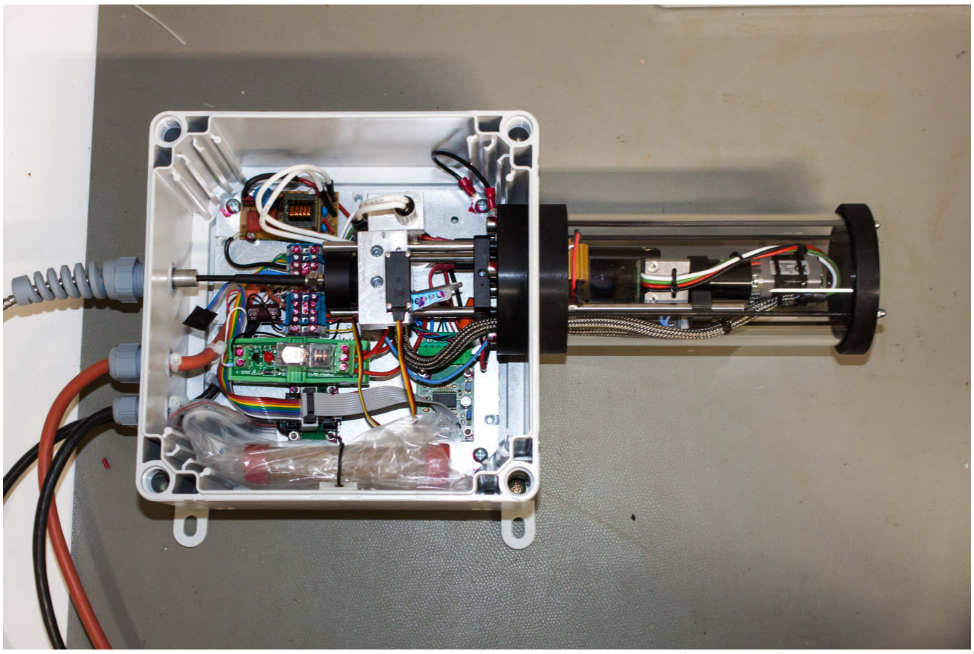


Figure 7: The Airyx SkySpec telescope scanner unit with HG-lamp and shutter

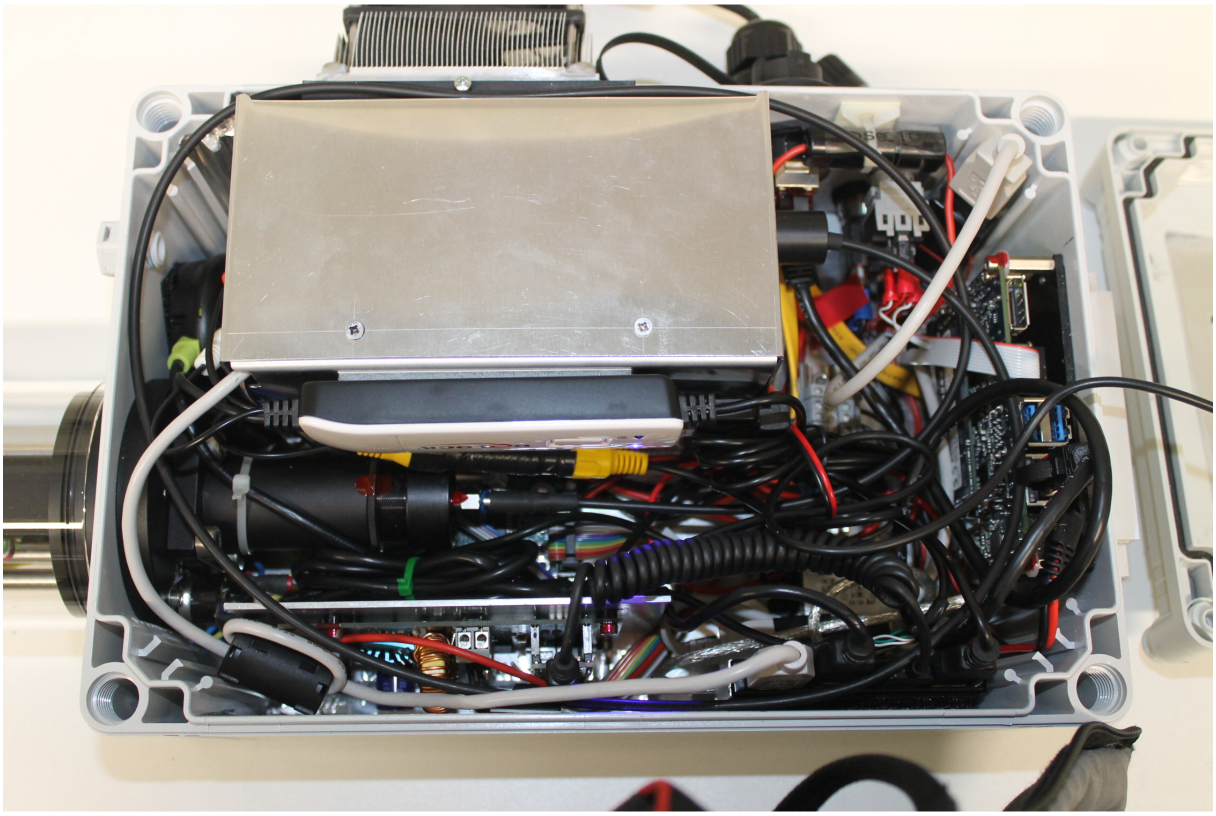


Figure 8: The Airyx SkySpec-mini instrument with one spectrometer. The interior is packed a lot denser than for the other instruments. The embedded PC can be found on the right, on top the slot for the adapter for an external display is found.

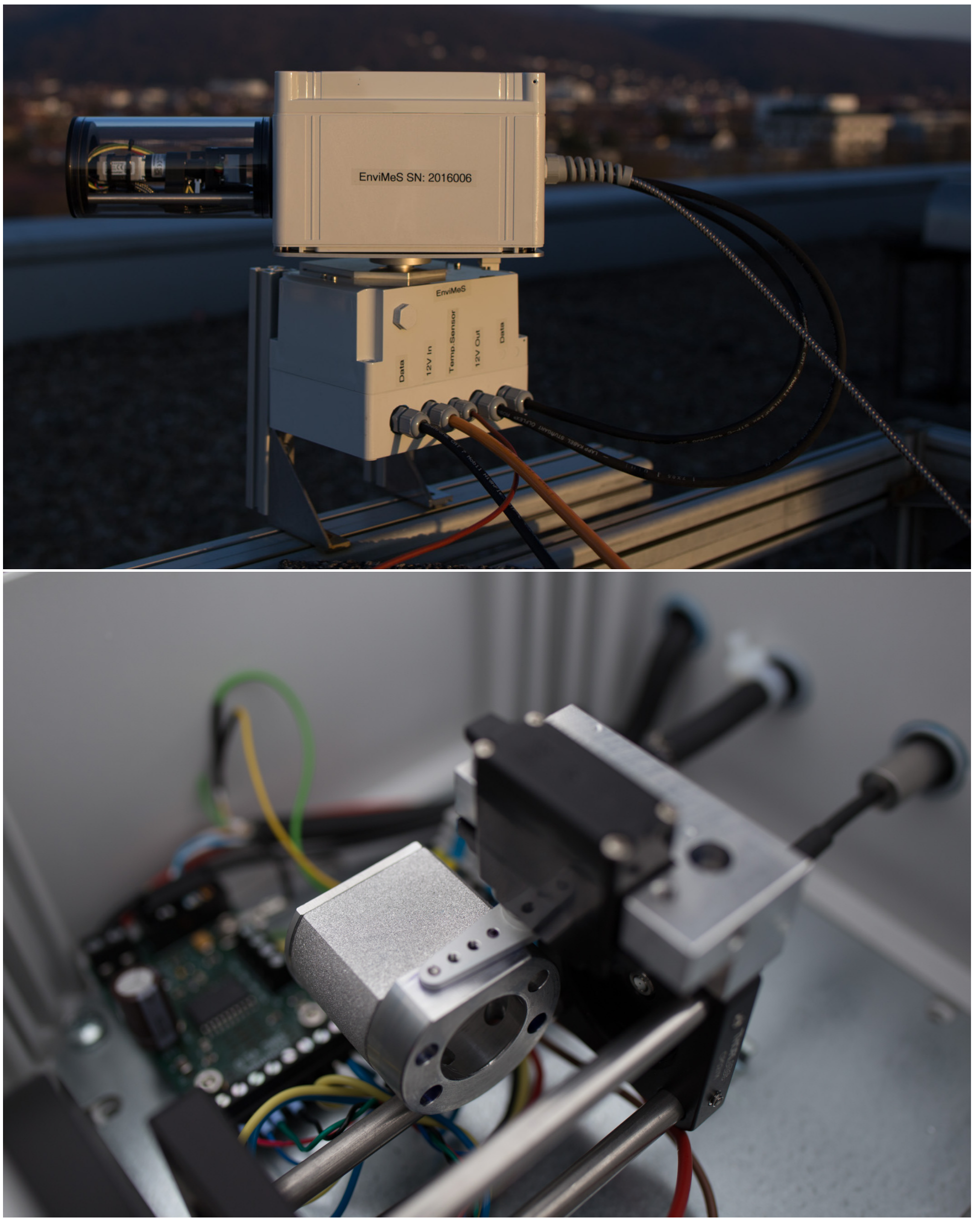


Figure 9: 2D telescope scanner unit. Below: Diffuser of the 2D unit. Be aware that the fibre needs move freely for all telescope positions and is not fixed at any point. Here the fibre was led over an additional aluminium rod to the ground (not on the picture).

Bibliography

[Aliwell et al., 2002] Aliwell, S. R., Van Roozendael, M., Johnston, P. V., Richter, A., Wagner, T., Arlander, D. W., Burrows, J. P., Fish, D. J., Jones, R. L., Tørnkvist, K. K., Lambert, J.-C., Pfeilsticker, K., and Pundt, I. (2002). Analysis for bro in zenith-sky spectra: An intercomparison exercise for analysis improvement. *Journal of Geophysical Research: Atmospheres*, 107(D14):ACH 10–1–ACH 10–20.

[Bogumil et al., 2003] Bogumil, K., Orphal, J., Homann, T., Voigt, S., Spietz, P., Fleischmann, O., Vogel, A., Hartmann, M., Bovensmann, H., Frerik, J., and Burrows, J. (2003). Measurements of molecular absorption spectra with the SCIAMACHY pre-flight model: Instrument characterization and reference data for atmospheric remote-sensing in the 230-2380nm region. *J. Photochem. Photobiol. A.*, 157:167–184.

[Bussemer, 1993] Bussemer, M. (1993). Der Ring- Effekt: Ursachen und Einfluß auf die spektroskopische Messung stratosphärischer Spurenstoffe. Diploma thesis, Heidelberg University, Heidelberg, Germany.

[Chance and Kurucz, 2010] Chance, K. and Kurucz, R. (2010). An improved high-resolution solar reference spectrum for earth's atmosphere measurements in the ultraviolet, visible, and near infrared. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111(9):1289 – 1295. Special Issue Dedicated to Laurence S. Rothman on the Occasion of his 70th Birthday.

[Chance and Orphal, 2011] Chance, K. and Orphal, J. (2011). Revised ultraviolet absorption cross sections of H_2CO for the HITRAN database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 112(9):1509 – 1510.

[Dinter et al., 2015] Dinter, T., Rozanov, V. V., Burrows, J. P., and Bracher, A. (2015). Retrieving the availability of light in the ocean utilising spectral signatures of vibrational raman scattering in hyper-spectral satellite measurements. *Ocean Science*, 11(3):373–389.

[Fleischmann, 2004] Fleischmann, O. (2004). New ultraviolet absorption cross-sections of BrO at atmospheric temperatures measured by time-windowing fourier transform spectroscopy. *Journal of Photochemistry and Photobiology A: Chemistry*, 168:117–132.

[Fry et al., 1992] Fry, E. S., Kattawar, G. W., and Pope, R. M. (1992). Integrating cavity absorption meter. *Appl. Opt.*, 31:2055–2065.

[Greenblatt et al., 1990] Greenblatt, G. D., Orlando, J. J., Burkholder, J. B., and Ravishankara, A. R. (1990). Absorption measurements of oxygen between 330 and 1140 nm. *J. Geophys. Res.*, 95:18577–18582.

[Hermans et al., 1999] Hermans, C., Vandaele, A. C., Carleer, M., Fally, S., Colin, R., Jenouvrier, A., Coquart, B., and Mérienne, M.-F. (1999). Absorption cross-sections of atmospheric constituents: NO_2, O_2, and H_2O. *Environ. Sci. & Pollut. Res.*, 6(3):151–158.

[Kraus, 2006] Kraus, S. (2006). *DOASIS - A Framework Design for DOAS*. Dissertation, Heidelberg University.

[Kromminga et al., 2003] Kromminga, H., Orphal, J., Spietz, P., Voigt, S., and Burrows, J. (2003). New measurements of oclo absorption cross-sections in the 325-435 nm region and their temperature dependence between 213 and 293 k. *Journal of Photochemistry and Photobiology A: Chemistry*, 157(2):149 – 160. Atmospheric Photochemistry.

[Lampel et al., 2015a] Lampel, J., Frieß, U., and Platt, U. (2015a). The impact of vibrational raman scattering of air on doas measurements of atmospheric trace gases. *Atmospheric Measurement Techniques*, 8(9):3767–3787.

[Lampel et al., 2017] Lampel, J., Pöhler, D., Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., Tennyson, J., Lodi, L., Frieß, U., Wang, Y., Beirle, S., Platt, U., and Wagner, T. (2017). Detection of water vapour absorption around 363 nm in measured atmospheric absorption spectra and its effect on doas evaluations. *Atmospheric Chemistry and Physics*, 17(2):1271–1295.

[Lampel et al., 2015b] Lampel, J., Pöhler, D., Tschritter, J., Frieß, U., and Platt, U. (2015b). On the relative absorption strengths of water vapour in the blue wavelength range. *Atmospheric Measurement Techniques*, 8(10):4329–4346.

[Peters et al., 2014] Peters, E., Wittrock, F., Richter, A., Alvarado, L. M. A., Rozanov, V. V., and Burrows, J. P. (2014). Liquid water absorption and scattering effects in doas retrievals over oceans. *Atmospheric Measurement Techniques*, 7(12):4203–4221.

[Puķīte et al., 2010] Puķīte, Janis, J., Kühl, S., Deutschmann, T., Platt, U., and Wagner, T. (2010). Extending differential optical absorption spectroscopy for limb measurements in the UV. *Atmospheric Measurement Techniques*, 3(3):631–653.

[Rothman et al., 2013] Rothman, L., Gordon, I., Babikov, Y., Barbe, A., Benner, D. C., Bernath, P., Birk, M., Bizzocchi, L., Boudon, V., Brown, L., Campargue, A., Chance, K., Cohen, E., Coudert, L., Devi, V., Drouin, B., Fayt, A., Flaud, J.-M., Gamache, R., Harrison, J., Hartmann, J.-M., Hill, C., Hodges, J., Jacquemart, D., Jolly, A., Lamouroux, J., Roy, R. L., Li, G., Long, D., Lyulin, O., Mackie, C., Massie, S., Mikhailenko, S., Müller, H., Naumenko, O., Nikitin, A., Orphal, J., Perevalov, V., Perrin, A., Polovtseva, E., Richard, C., Smith, M., Starikova, E., Sung, K., Tashkun, S., Tennyson, J., Toon, G., Tyuterev, V., and Wagner, G. (2013). The HITRAN2012 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 130(0):4 – 50. HITRAN2012 special issue.

[Rothman et al., 2010] Rothman, L., Gordon, I., Barber, R., Dothe, H., Gamache, R., Goldman, A., Perevalov, V., Tashkun, S., and Tennyson, J. (2010). HITEMP, the high-temperature molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111(15):2139 – 2150. XVIth Symposium on High Resolution Molecular Spectroscopy (HighRus-2009).

[Serdyuchenko et al., 2014] Serdyuchenko, A., Gorshelev, V., Weber, M., Chehade, W., and Burrows, J. P. (2014). High spectral resolution ozone absorption cross-sections - part 2: Temperature dependence. *Atmospheric Measurement Techniques*, 7(2):625–636.

[Sihler et al., 2016] Sihler, H., Lübcke, P., Lang, R., Beirle, S., de Graaf, M., Dörner, S., Hörmann, C., Lampel, J., de Vries, M. P., Poli, G., Remmers, J., Trollope, E., Wang, Y., and Wagner, T. (2016). Discrete field of view sampling/retrieval using high-resolution imager data – applied on gome-2 and omi satellite and so2-camera instruments. *Atmospheric Measurement Techniques.*

[Spietz et al., 2005] Spietz, P., Gómez Martín, J. C., and Burrows, J. P. (2005). Spectroscopic studies of the I_2/O_3 photochemistry: Part 2. improved spectra of iodine oxides and analysis of the IO absorption spectrum. *Journal of Photochemistry and Photobiology A: Chemistry*, 176(1-3):50 – 67. In Honour of Professor Richard P. Wayne.

[Stutz et al., 2000] Stutz, J., Kim, E. S., Platt, U., Bruno, P., Perrino, C., and Febo, A. (2000). UV-visible absorption cross sections of nitrous acid. *Journal of Geophysical Research*, 105(D11):14585.

[Stutz and Platt, 1996] Stutz, J. and Platt, U. (1996). Numerical analysis and estimation of the statistical error of differential optical absorption spectroscopy measurements with least-squares methods. *Appl. Opt.*, 35(30):6041–6053.

[Thalman and Volkamer, 2013] Thalman, R. and Volkamer, R. (2013). Temperature dependent absorption cross-sections of O_2–O_2 collision pairs between 340 and 630 nm and at atmospherically relevant pressure. *Physical Chemistry Chemical Physics*, 15(37):15371–15381.

[Vandaele et al., 1998] Vandaele, A., Hermans, C., Simon, P., Carleer, M., Colin, R., Fally, S., Merienne, M., Jenouvrier, A., and Coquart, B. (1998). Measurements of the NO_2 absorption cross-section from 42 000 cm^{-1} to 10 000 cm^{-1} (238-1000 nm) at 220 K and 294 K. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 59(3-5):171 – 184. Atmospheric Spectroscopy Applications 96.

[Vandaele et al., 2009] Vandaele, A. C., Hermans, C., and Fally, S. (2009). Fourier transform measurements of so 2 absorption cross sections: Ii.: Temperature dependence in the 29000–44000cm- 1 (227–345nm) region. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 110(18):2115–2126.

[Vogel et al., 2013] Vogel, L., Sihler, H., Lampel, J., Wagner, T., and Platt, U. (2013). Retrieval interval mapping: a tool to visualize the impact of the spectral retrieval range on differential optical absorption spectroscopy evaluations. *Atmospheric Measurement Techniques*, 6(2):275–299.

[Volkamer et al., 2005] Volkamer, R., Spietz, P., Burrows, J. P., and Platt, U. (2005). High-resolution absorption cross-section of glyoxal in the UV/vis and IR spectral ranges. *J. Photoch. Photobio. A: Chemistry*, 172:35 – 46.

[Wagner et al., 2009] Wagner, T., Deutschmann, T., and Platt, U. (2009). Determination of aerosol properties from MAX-DOAS observations of the Ring effect. *Atmospheric Measurement Techniques*, 2(2):495–512.

[Wenig et al., 2005] Wenig, M., Jähne, B., and Platt, U. (2005). Operator representation as a new differential optical absorption spectroscopy formalism. *Applied optics*, 44(16):3246–3253.