The University of Melbourne
School of Earth Sciences

UniMelb EnviMeS MAX-DOAS users guide

A supplement to the EnviMeS manual, for Aurora Australis voyages, summer 2017/2018

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Contents

1 Introduction to MAX-DOAS

Multi-axis differential optical absorption spectroscopy (MAX-DOAS) is a UV-Visible spectroscopic technique with the ability to provide vertical profile information on aerosol parameters and various atmospheric trace gases. Analysis trace gases of interest include ozone, nitrogen dioxide, formaldehyde, glyoxal and bromine monoxide.

The term *differential optical absorption* refers to the spectroscopic analysis technique which allows the Beer-Lambert law for light attenuation through an absorber, to be applied in an atmospheric context. More on this can be found in the "Quick introduction to DOAS data processing" section at the end of this document. DOAS can either be *active*, using a synthetic light source (such as a laser or LED) or *passive*, using a natural light source (such as the sun). *Multi-axis* DOAS is an example of a passive remote sensing DOAS instrument, measuring solar spectra at a series of different elevation angles. When referenced against a 90^o (zenith) scan, spectra from the low elevation angles with respect to the horizon contain information about the boundary layer and lower troposphere. This is illustrated in figure 1.

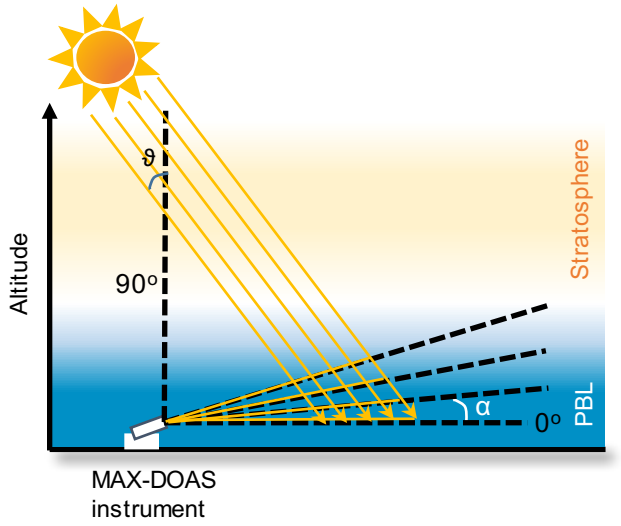

Figure 1: Simple MAX-DOAS geometry showing the elevation angle (α) and solar zenith angle (θ) relative to the detector and the sun, respectively. Observations at low elevation angle provide long path lengths through the planetary boundary layer (PBL) while having the same path through the stratosphere.

The MAX-DOAS instrument consists of two main parts. Firstly a telescope box houses the optics for receiving sunlight, and a small stepping motor which varies the elevation angle. Secondly, a fibre optic cable connects the telescope optics to a spectrometer box, containing two cooled Avantes spectrometers (one in the UV range, 300-450 nm, one in the visible range, 405-560 nm). A laptop computer records and collects the spectra for processing and analysis.

The UniMelb MAX-DOAS instrument was built by the Environmental Measurement Systems company (EnviMeS) in Heidelberg, Germany. It comes with data collection software MS-DOAS and spectral viewing/processing software DOASIS. The following section sets out important information for the safe operation of the MAX-DOAS which should be read alongside the EnviMeS manual.

2 The MAX-DOAS instrument

2.1 Spectrometer box

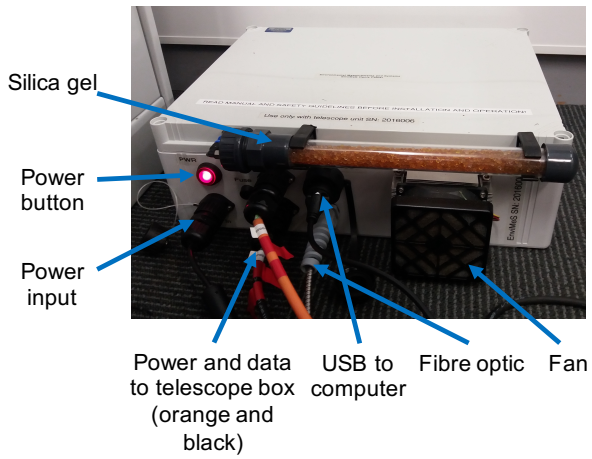

Figure 2: The MAX-DOAS spectrometer box

- The spectrometer box needs to stay indoors. Connecting cables include power, USB connection to the computer, and power, data and fibre-optic connections to the telescope box. The data and power cables to the spectrometer box need to be connected during operation. The plug shapes make it impossible to connect the cables in the wrong place.
- **The fibre optic (silver cable) is not to be disconnected from the spectrometer box, only remove from the telescope box end.**
- **Temperature control:** the spectrometer needs to be kept at an internal temperature of 20^oC at all times during operation. This is monitored in the MS-DOAS software (more on this in the software section of this document). It is important to monitor this routinely (i.e. at least once a day) during operation.
- **Silica gel:** The spectrometer box needs to stay dry inside. The tube of orange silica gel desiccant on the outside of the box ensures this is the case. If this silica gel starts to turn blue/green it will need to be changed. The following procedure should be followed:
  1. Stop all devices in MS-DOAS (see figure 5)
  2. Close MS-DOAS and power off the spectrometer box
  3. With your left hand, hold the round screw-in connector at the power button end, while unscrewing the attached hexagonal connector. Do not twist the round end as this is connected to the air inlet tube.
  4. When these pieces are unscrewed, carefully prise the glass tube from the holders
  5. Replace the silica gel
  6. Reverse steps 1 to 4 and restart the instrument

2.2 Telescope box

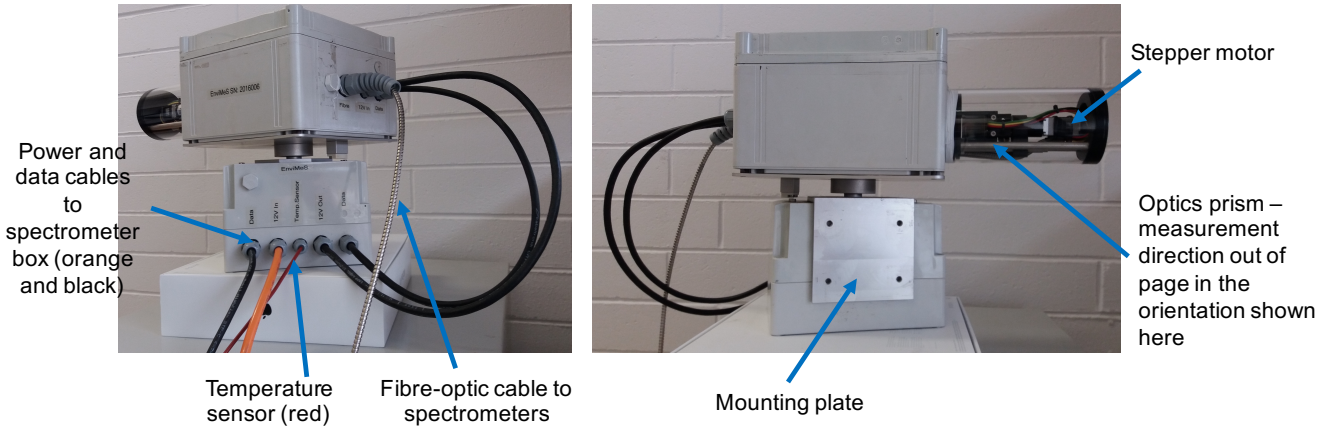

Figure 3: Images of the MAX-DOAS telescope box

- The orange and black data and power cables are not to be removed from the telescope box. Only the silver fibre optic cable is to be removed upon pack-down.
- **Fibre optic cable:** Great care must be taken with connecting the optical fibre to the telescope unit. The following procedure should be followed:
  1. Remove the lid of the telescope box (a large flathead screwdriver will remove the crossed screws)
  2. Unscrew the grey plastic curly housing from telescope unit
  3. Put this plastic piece over the fibre and push it down out of the way for the moment
  4. Put the fibre through the back of the telescope unit and through the rubber sealing. Do not pull on the end of the fibre, only push the thick silver part. The seal is very tight so the process is fiddly, requiring strong fingers and even stronger patience. Don't rush!
  5. Keep pushing until the end of the fibre is close to the optics hole. Then remove the black cap on the tip of the fibre
  6. Gently keep sliding the fibre through by pushing the thick silver part from outside the box, or pulling only(!) the thick silver bit that has made it inside the box. It should line up so that the fibre tip goes into the optics hole
  7. Once the fibre is all the way in, the silver fibre screw connector can be tightened. If you can't get the screw cap to engage or tighten, the fibre isn't in far enough
  8. On the outside of the box, screw the grey curly plastic housing back on over the place where the fibre enters the box
  9. Screw the lid of the box back on and you're done
- **Silica gel:** Being outside, the telescope box is vulnerable to sea-spray, rain and pressure changes which can cause moisture to condense inside the box and the telescope. Sometimes condensation is obvious to the naked eye through the telescope glass. There is a silica gel pack inside the telescope box which will need to be checked at regular intervals. Not having run it

on a ship yet, I would suggest once every two days (if it isn't raining/heavy seas/dangerous to go outside!) at least until you are familiar with how long the silica gel will actually last. To change the desiccant, follow the following procedure:

1. Stop all devices in MS-DOAS (see figure 5)
2. Close MS-DOAS and power off the spectrometer box
3. Unscrew the lid of the telescope box using a large phillips or flat-head screwdriver. The screwdriver needs to be large in order to avoid damaging the plastic screws.
4. Remove the whole desiccant tube from the adjustable zip-tie holder and replace the silica gel
5. Reverse steps 1-4, taking care to put the lid back in the same orientation you took it off, because otherwise the desiccant tube can hit the optics.

- **Cleaning the telescope:** at sea, spray and salt may build up on the outside of the telescope. This can be cleaned by flushing the outside of the telescope with water and/or wiping with a non-scratching damp cloth.
- **Fixed azimuth motor component:** this MAX-DOAS has an azimuth motor which rotates the upper part of the spectrometer box laterally. For the Aurora voyages this function has been disabled completely in the firm- and software, and we are relying on a pin. The pin is tightened through a white nylon block from the base-plate of the upper telescope box to the mounting bracket of the lower telescope block. On the ship, it is crucial that the azimuth component isn't allowed to rotate or swing all all so it will be important to regularly check this by hand and tighten the screw if required.
- **Items added inside telescope box:** For this voyage, an accelerometer and USB-GPS dongle have been added (see sections below). To accomodate this, a USB connection and 4-port usb hub have been added. The 4-port hub and accelerometer have been stuck down inside the box with velcro tape. It will be a good idea to check that these components are still firmly in place during the Aurora voyages, when the silica gel is checked.

3 Extra hardware

3.1 Camera

A camera has been configured to run with the MAX-DOAS data collection software. This is actually a re-purposed car reversing camera, connected to the laptop using a S-video to USB adapter. Opening the MS-DOAS software (see software section below) will allow the camera to be turned on to check the generated image quality. It may be necessary to check the camera for salt/sea spray/other dust during the voyage.

3.2 Accelerometer

A small portable accelerometer has been added inside the telescope box (see figure 4). This instrument is logging the Euler angles corresponding to pitch, roll and yaw. The MAX-DOAS controlling

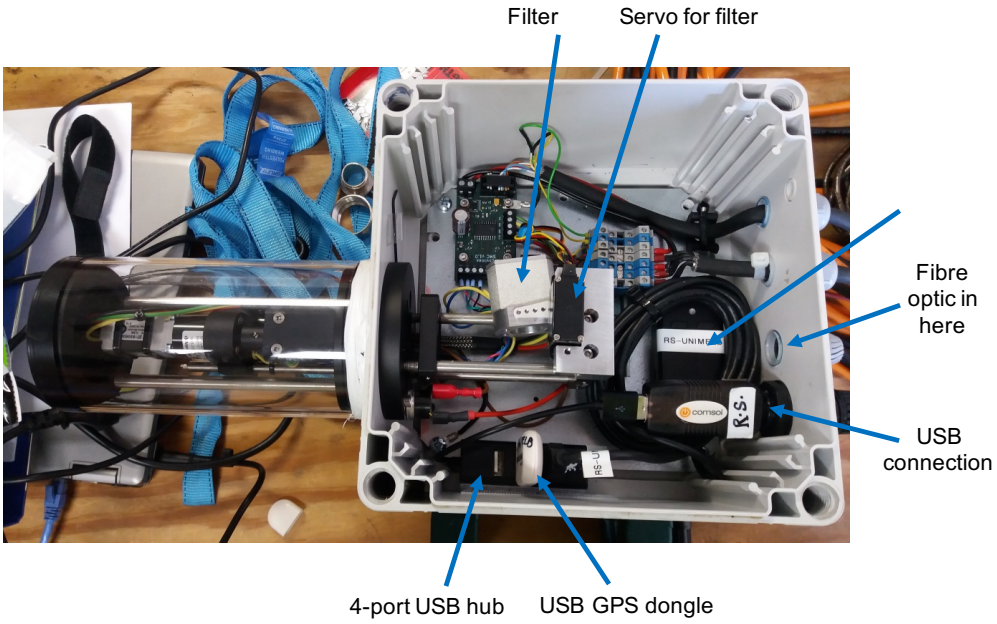

Figure 4: Image of the inside of the MAX-DOAS telescope box, before fibre-optic cable has been connected

software, MS-DOAS, is not configured to collect this data so accelerometer log files are generated in a separate software called "3-Space Suite".

To log data in 3-Space, select Data Charts in the bottom right hand corner of the main interface. "Logging options" in the bottom right corner of the Data Charts window allows the data path to be updated. Make sure the DateTime timestamp option is selected and ASCII data format. Once these options are set, click "Start logging". The pitch, roll and yaw data are updated approximately every 10 microseconds. This frequency is higher than needed and currently unable to be changed. Therefore the data can be resampled using a Python script to reduce the size of the accelerometer files to be saved.

Since MAX-DOAS measurements only occur during daylight hours, the accelerometer data during the night is not needed. To save hard-drive file space the logging could be stopped in the night (so long as it is restarted before sunrise) or alternatively the logging stopped once a day, and the night-time data manually removed.

3.3 GPS

The measurement software operates on a timing sequence which relies on knowing the solar position. Since measurements rely on sunlight, measurements are programmed to cease when the solar zenith angle (SZA, angle of the sun in sky relative to the zenith) is greater than 90 - i.e. when the sun is below the horizon. Since sunset time will vary considerably over the course of the distance between Tasmania and Antarctica, an external USB-GPS system is required to continuously update the latitude and longitude.

The GPS should appear under a COM port in the Windows Device Manager. If it appears as a "location sensor" instead, the driver software will need to be rolled back to the previous version (this can be done under the device Properties in the Windows Device Manager). Outside of using

the GPS in MS-DOAS, the GPS receiver can be tested using the U-center software on the MAX-DOAS laptop. In U-center, use the "connect" button (top left) to connect to the appropriate COM port and then select the Baud rate as 57600. Once connected, the satellites the GPS is fixed on should appear in the windows on the right hand side, and the latitude and longitude should update in the data panel on the far right. Failure to connect to a satellite may result if the GPS receiver is too close to electromagnetic sources (such as other computers).

4 Software

4.1 MS-DOAS

MS-DOAS is the software written by EnviMeS for controlling the MAX-DOAS instrument. A screenshot of the main interface is in figure 5. Each of the components of the system are controlled by a tab in the menu panel on the left hand side of the interface and can be accessed by double clicking on the name. Each component can be configured by hitting the wheel-like button in the top left of the tab.

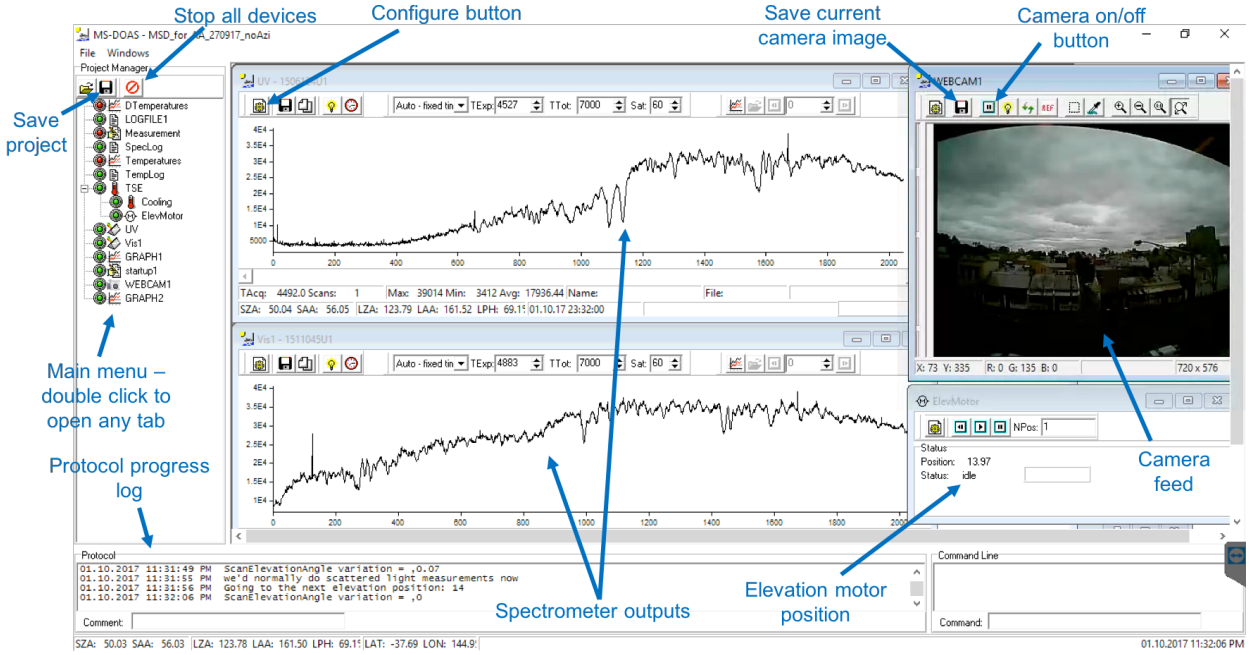

Figure 5: Screenshot of the MS-DOAS main interface when the instrument is in operation

4.1.1 Starting MS-DOAS

MS-DOAS can be opened by clicking on the icon shown in figure 6, or the desktop icon "MS-DOAS Shortcut" (not "MS-DOAS shortcut new").

Upon startup, all the tabs in the project file will open and flash up. In the protocol progress log in the bottom left, messages should appear saying that connection to the two spectrometers and the TSE stepper has been successful. If connection to the TSE stepper is not successful, try

Figure 6: Screenshot of the laptop's toolbar showing the MS-DOAS icon to open

closing MS-DOAS, powering off the spectrometer, disconnecting and then reconnecting all cable connections to the spectrometer box (except the fibre-optic).

If connection to the spectrometers is not successful, open the spectrometer configuration menu which will look like the image in figure 8. From the drop down menu choose the correct Avantes serial number as shown in the image. If this does not solve the problem, try closing MS-DOAS, powering off the spectrometer, disconnecting and then reconnecting all cable connections to the spectrometer box (except the fibre-optic).

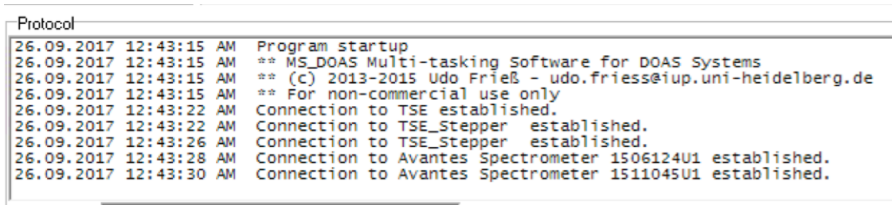

Figure 7: Screenshot of the MS-DOAS protocol log, showing display after correct program startup and loading of the TSE and spectrometer components

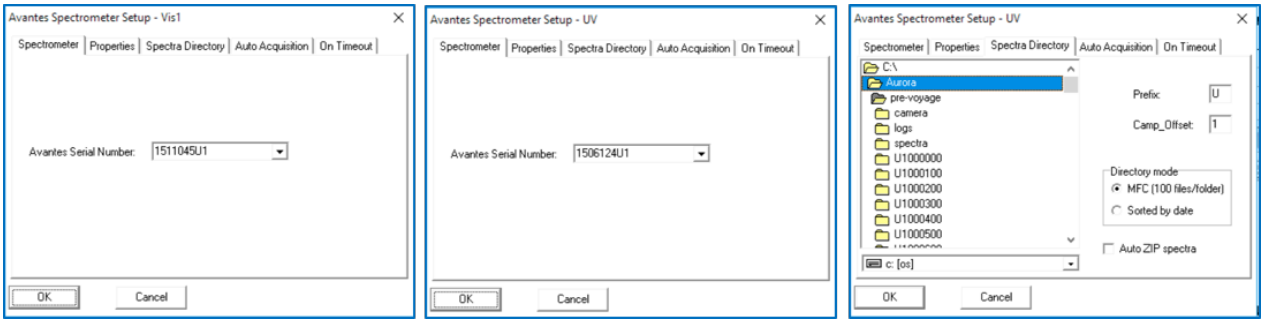

Figure 8: Screenshot of the MS-DOAS spectrometer configuration tab, showing the correct Avantes serial numbers for each spectrometer, and example saving directory set up.

4.1.2 Things to check before beginning measurements

- **Spectral saving directory** - check that spectra are saving in the correct directory by opening the configuration tabs for both spectrometers and checking the directory as shown in figure 8
- **Camera connection** - The external camera is called "Webcam1" in the MS-DOAS project. Check in the Webcam1 configuration tab that the 'device' is set to the external USB device rather the computer's inbuilt webcam. Also check that the camera images are being saved in the correct directory. The camera configuration tab is shown in figure 9

- **Camera test** - the camera has an image menu which is on the left hand side of the image (drag the image to the right to find the menu). In this menu the brightness, saturation, sharpness and other parameters can be optimised for the light conditions, to ensure best possible image quality
- **GPS receiver** - using the configure button in the top left of the GPS tab, select the appropriate COM port (this can be found in the Windows Device Manager under COM ports), the Baud rate 57600 and tick the box to update the geolocation. If the GPS can't update latitude and longitude, the receiver may need to shifted until a connection can be established. The actual satellites the receiver is trying to connect to can be viewed in the U-center software. Note that only one of U-center or MS-DOAS can access the COM port at once, so close one software if trying to use the GPS in the other.

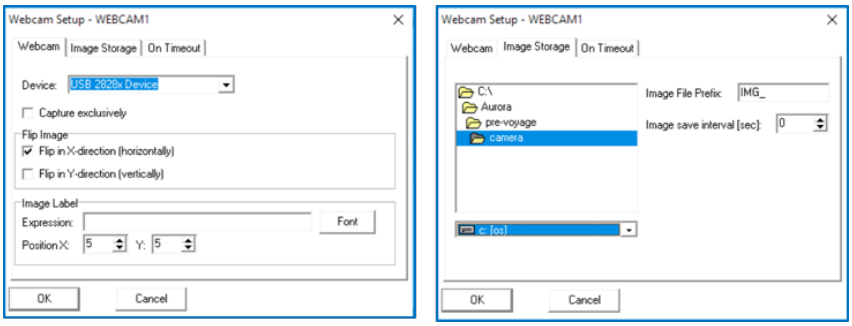

Figure 9: Screenshot of the MS-DOAS camera configuration tab.

4.1.3 Measurement startup

Measurements can be started by opening the "startup1" tab and clicking the start button as shown in figure 10. A series of initialisation commands are carried out to set the elevation motor position, test the camera connection and temperature controls. The message "Measurements ready to start" appearing will indicate that the initialisation has occurred successfully.

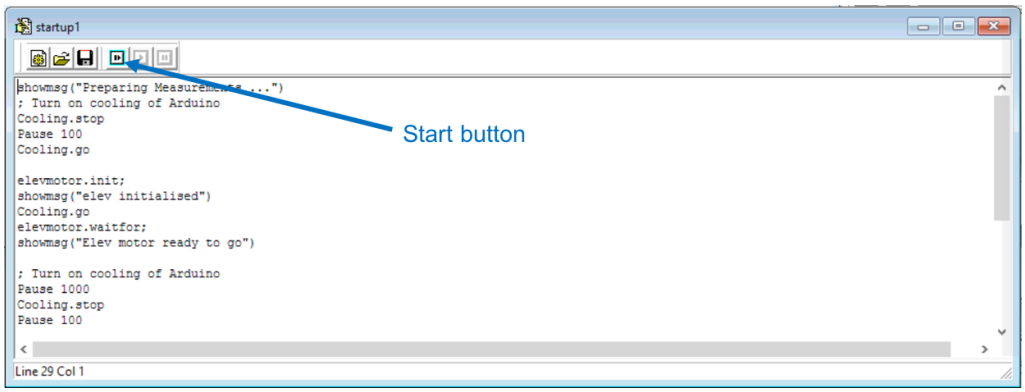

Figure 10: Screenshot of the MS-DOAS startup tab, showing how to start measurement sequence

4.1.4 Things to check when measurements start

Once measurements start, minimise the "startup" tab so that the MS-DOAS interface looks like figure 5.

- **Spectra** - check that spectra are being recorded in both the UV and Vis spectra tabs. In daylight, the spectra should look like those in figure 5. The MS-DOAS file saving structure for spectra is an 8 character code - e.g. U1000100 for the UV spectrometer and V1000100 for the vis spectrometer. Files are saved in directories with 100 files to a folder.
- **Elevation motor tab** - check that the elevation position varies with each scan. The exact sequence of elevation angles (EAs) is listed in the "Measurement" tab. The "name" of each spectrum is recorded in the bottom of the spectra tab, showing the set EA, the actual EA at the start of the scan and the actual EA at the end of the scan. Ideally these values should all be similar (i.e. within 0.1), but the consistency may vary under rough sea conditions.
- **Temperatures** - the temperature is logged in the "templog" tab and plotted in the "Temperatures" tab (see figure 11. The spectrometer is cooled and must be at 20^{o}C, check this daily. The other temperatures can vary.
- **Camera** - the camera cannot remain on all the time due to computer memory issues. When scans begin you should see the camera feed pause and restart each scan.
- **Calibrations** - dark calibration measurements are programmed to run during the night (usually about 1 hour after sunset). There are two types of calibration measurements. Dark current calibrations have a long exposure time (approx. 30 seconds) while offset calibrations have short exposure time (approx 3 ms) but a large number of scans. These are only required for later data evaluation and should not need any additional attention during the voyages.

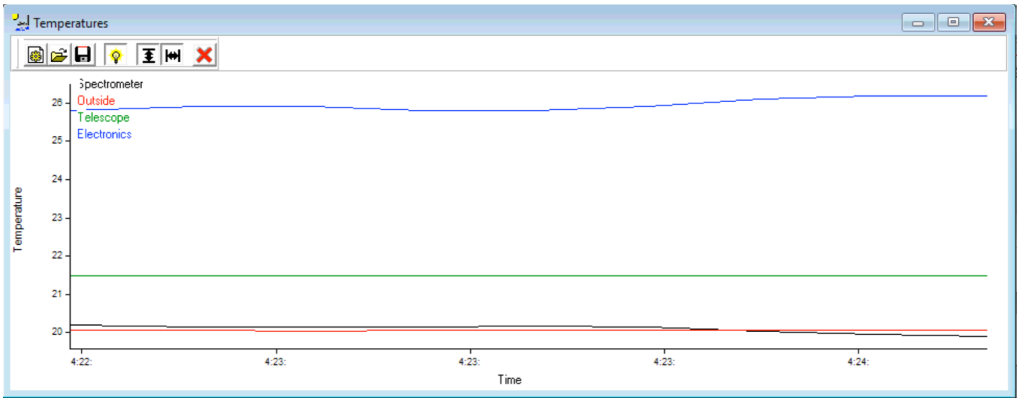

Figure 11: Screenshot of the MS-DOAS temperature log plot. The black line (spectrometer temperature) should not deviate more than 1^{o}C from 20^{o}C.

4.2 DOASIS

DOASIS is software designed for browsing and analysing spectra. It is designed to open text files, binary spectra files (such as from MS-DOAS) and ASCII standard (.std) spectral files. DOASIS can be opened using the taskbar icon shown at the bottom of figure 12. The best way to open and browse spectra in DOASIS is to click on the "open sequential" button as shown in figure 12, and

navigate to the directory of interest. This is a good way, for example, to look over spectra and see if there are any/many with elevation angles varying significantly from the nominal value.

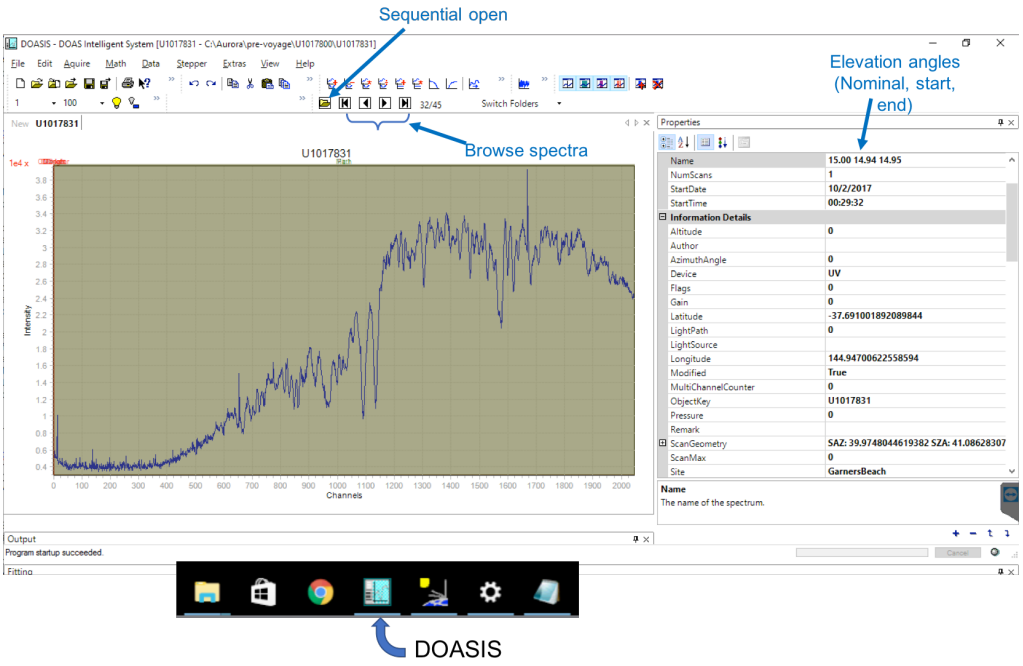

Figure 12: Screenshot of the DOASIS main interface, with a spectrum opened.

4.3 Using DOASIS to convert spectra to .std

Further analysis of spectra using external analysis tools requires the conversion of MS-DOAS binary spectra to .std files (an ASCII format, one spectrum per file). Note: in order to send spectral files back from the Aurora, it is recommended to send the raw MS-DOAS binary files NOT the .std files since the binary files are 9 kb per spectrum, while the .std files are 16 kb per spectrum.

The process to do the conversion is outlined here:

1. Open the "script" window, as shown in figure 13(a)
2. Open the javascript code "`save_to_std_master.js`" (this needs to be saved in the folder where the binary file directories are stored). Update the number of the first and last files to be converted, and "U" or "V" depending on whether UV or Visible files are to be converted, as shown in figure 13(b). Save the file after modifications.
3. In the DOASIS script window (figure 13(c)), navigate to the updated "`save_to_std_master.js`" script. Then select "start". The code should run. If an error "file not found" appears, check again that the code is saved in the right place and with the right start and end file numbers.

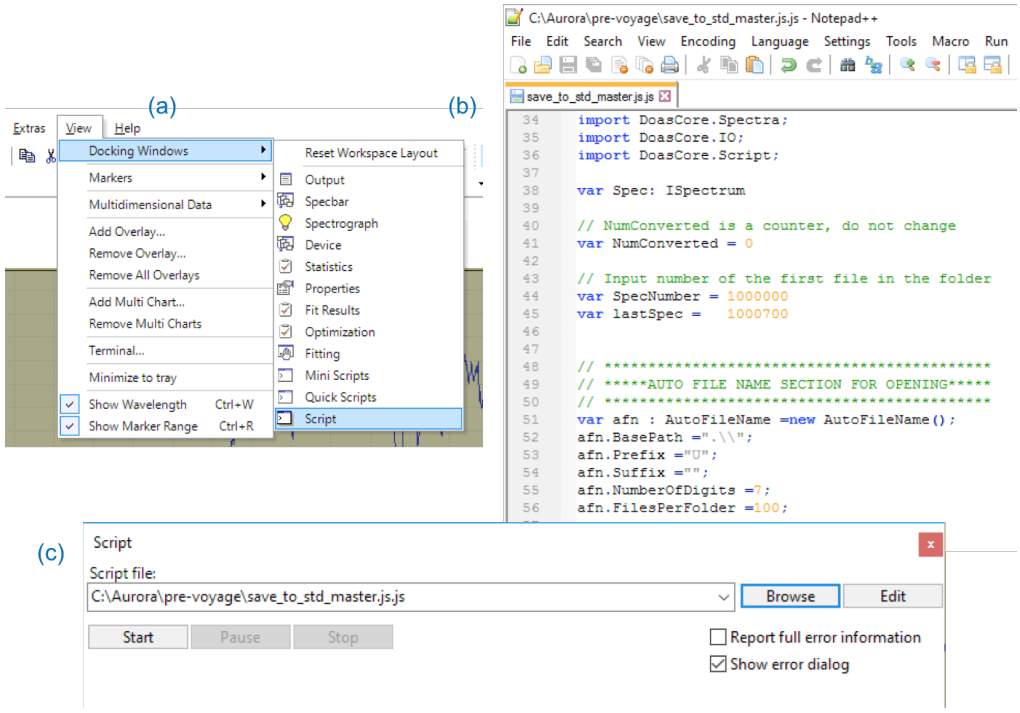

Figure 13: Screenshot of the DOASIS menus and javascript code required to convert MS-DOAS binary files to ASCII .std files.

5 Daily check

The points below comprise a daily check for the MAX-DOAS while in operation;

- Record date, time (UTC), solar zenith angle, latitude, longitude, spectrum number and spectrum name when the daily check is begun
- Date and time on laptop matches ship's time (UTC)
- Latitude and longitude from USB-GPS match ship's log
- Record weather conditions at the time of the daily check
- Telescope wiped clean of salt/sea-spray/rain/other dirt
- Telescope box silica gel ok? (Check at least twice weekly)
- Azimuth turning component of telescope box is firmly fixed, pin screw holding this in place tightened if not
- GPS is updating latitude and longitude
- Spectra are being recorded, elevation angle sequence being followed
- Accelerometer is outputting data and logging through 3-Space software, daily data saved
- Camera is operational, is saving images
- Spectrometer temperature 20^{o}C

- Spectra from previous day converted to .std files in DOASIS
- Spectra from previous day backed up
- Spectra from previous day sent back to Melbourne

6 Inventory of MAX-DOAS items

- Spectrometer box with silver metal fibre optic cable attached. Out of operation, fibre optic should have small black cap over the end
- Telescope box with 10 m orange and black extension cables attached
- Power cable for telescope box
- Instrument DELL laptop and laptop charger
- USB data cable to connect spectrometer box to laptop
- Four port USB hub for laptop
- USB male to USB female 5 m cable for GPS to laptop
- U-Blox7 USB GPS receiver
- Reversing camera
- K-world DVD maker2 Serial to USB adapter for camera
- 12 V power supply for camera
- 10 m camera serial extension cable
- Spare silica gel container ("Labchem", yellow label)
- Spirit level and hand-held compass
- UniStrut mounting posts (20 cm long) and accompanying right-angle brackets with M6 screws
- White nylon block and accompanying screw for securing azimuth component
- Portable 1 TB hard drive in blue case, for data backups. Also contains disk image in case of laptop hard drive failure.