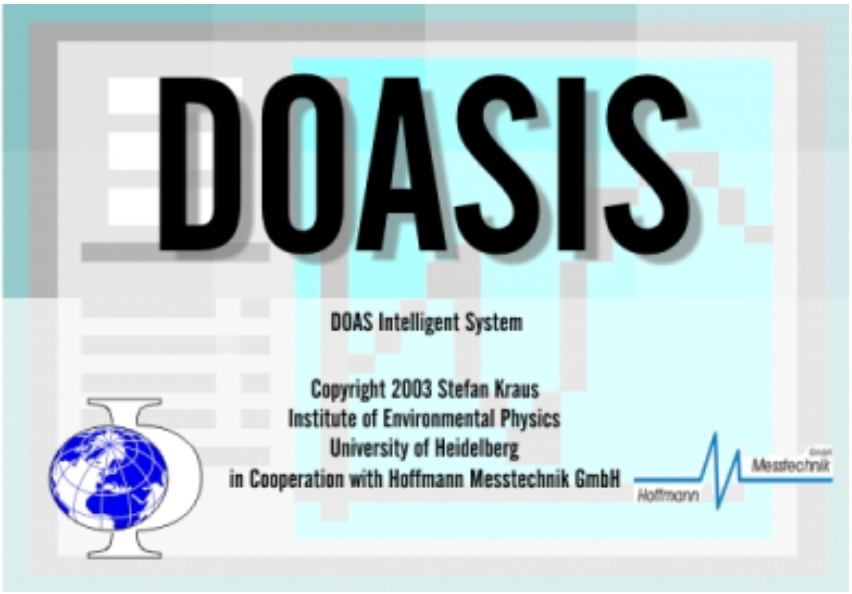
DOASIS Tutorial



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Contents

Chapter 1

Introduction

1.1 General Information

DOASIS is an all–round tool with which work with spectral data can be done. From acquiring to evaluation, everything can be done using the easy–to–use graphical user interface (GUI), which features:

- Tabbed Multiple Document Interface (MDI)
- Free floating docking windows for various kinds of toolboxes.
- Self–adapting menu structure (Office like menus)
- Shortcuts to various operations and hot–keys to quickly start user–defined scripts.
- Quick access to different kinds of operations using a floating toolbar.
- Support for Windows XP style settings.
- Full–featured support for modern multi user systems. Each user on a system can have his own settings that even propagate through domains automatically.
- Save the current programm state into a check point and restore it later to switch back to the original spectrum data.

Of course the functionality of the user interface can provide only basic operations. For more complex tasks the user must be able to define measurement or evaluation set–ups that fit best for his needs. Therefore DOASIS offers a scripting language called Jscript, which gives the user full control over the behaviour of the application and allows a fully automated usage. The script interface currently supports:

- JScript.NET language, which is based on JavaScript, an easy to learn programming language.
- Full access to all core functions of DOASIS including support of:
  - Spectra management: Create your own spectrum objects and manage them in collections.
  - Device control: Use several kinds of spectrographs, stepper motors, etc.
  - Mathematical support for spectral data.
  - I/O support to load and save a spectrum in various kinds of file formats.
  - Unified access to the user interface to communicate with the user from a scrip.

- Full asynchronous event handling model, so the user interface automatically recognizes changes made from a script to spectrum objects.
- Run a script in console mode without any graphical user interface. This feature can be used to run scripts on systems with little system resources where the GUI is "too heavy".
- Full debugging support of scripts using one of the .NET debuggers available.
- Script compiler instead of an interpreter to let scripts run with maximum performance.

All these features make DOASIS one of the most flexible applications suitable for anyone who needs to work with spectral data.

This tutorial of DOASIS introduces frequently used tasks in DOAS work. The Chapter 2 gives an overview of the graphical user interface and of some basic skills in handling spectra. Chapter 3 provides a complete description of all DOASIS menu points. In Chapter 4 the console windows will be explained, which also include some fitting examples. All properties and statistic items will be covered in Chapter 5. Since DOASIS can control different instruments, which use different methods to acquire spectra, Chapter 6 informs about the hardware that can be used and introduces some commonly used instruments (Acton spectrograph, HMT DOAS Controller and Ocean Optics).
For this tutorial it is assumed that DOASIS users are familiar with the basics of the DOAS technique.

1.2 Installing DOASIS

Minimum System Requirements:

- 200 MHz Pentium or compatible processor
- 64 MB RAM
- 60 - 100 MB hard disk space
- Microsoft Windows 98 or better (maybe later support for Linux)
- SVGA with a resolution of 800x600 at 16 colours
- Microsoft .NET Framework v1.1 or later (if this is not on your computer a link will automatically be given while installing DOASIS)

Recommended System Requirements:

- 500 MHz Pentium II or compatible processor
- 256 MB RAM
- 100 MB hard disk space
- Windows 2000 or better
- XSVGA with a resolution of 1280x1024 at 24 bit colour depth
- Microsoft .NET Framework SDK v1.1 or later (if this is not on your computer a link will automatically be given while installing DOASIS)

Installation package (you can choose which components shall be installed; all will be installed by default):

- Ocean Optics Library
- Solar Zenith Angle (SZA) calculation support
- Reference spectra

Since this is not yet the final version and minor changes might still be made, further updates and changes can be downloaded at:
http://www.iup.uni-heidelberg.de/institut/forschung/groups/atmosphere/software

1.3 Who can use DOASIS?

Commercial usage is not allowed without an explicit license grant from the author or the Institute of Environmental Physics. DOASIS is a non-commercial product that may be used by anyone else, but for scientific purpose only.

Chapter 2

First Steps

In this chapter DOASIS is presented to a novice user. The focus will be on basic skills of handling spectra that are already stored on disk, and to make best use of the graphical user interface. All tasks will be performed on exemplary spectra that will be provided by DOASIS so at this point DOAS hardware is not needed.

2.1 Starting DOASIS

To begin the tutorial, start DOASIS using the Windows start-menu. The DOASIS main window opens. On top of the DOASIS screen are the usual elements of a Windows-style program, i.e. a menu bar and tool buttons for fast access to frequently used menu functions. Use *file→open* or the tool-button to locate the demo Fraunhofer spectrum 'First_Example.spe' in the spectra folder within the DOASIS program folder. After opening it the spectrum is displayed on the spectrum sheet.
Now the key elements of the DOASIS screen, as shown below, are covered in detail.

2.2 Elements of the main screen

- *Spectrum sheets*: Spectrum sheets are used to display a graph of the spectrum data. The spectrum is plotted as a line graph in which the counts per detector channel are plotted against the channel (or wavelength) number. The count axis is scaled automatically to fit the plot area. *file→open* will display a new spectrum sheet, which is labeled with the spectrum's name or file name (for more on what exactly is meant by file and spectrum name see 3.1. The top spectrum sheet will be called the *active spectrum sheet* to which any kind of action concerning the alteration of spectra will apply exclusively.

- *Spec bar*: The Spec bar is an autonomous window, which holds thumbnail pictograms of all spectra that are currently open in a DOASIS session. Click on a thumbnail to display the selected spectrum in the active spectrum sheet. This can also be done by clicking on the spectrum sheet's name.

- *Information window*: The Information window consists of three sheets: statistics, properties and fit results. In the statistics sheet e.g. minimum, maximum and average count of the active spectrum are displayed. The properties sheet contains a lot of information about the spectra such as file information (file name etc.), markers & display and scan parameters, whereas the fit results sheet shows information of realized fits. For a more detailed description of the information window see 5.

- *Console window*: the console window consists of several sheets as well: the console sheet displays the running status of the program (e.g. running scripts etc.), the dif-

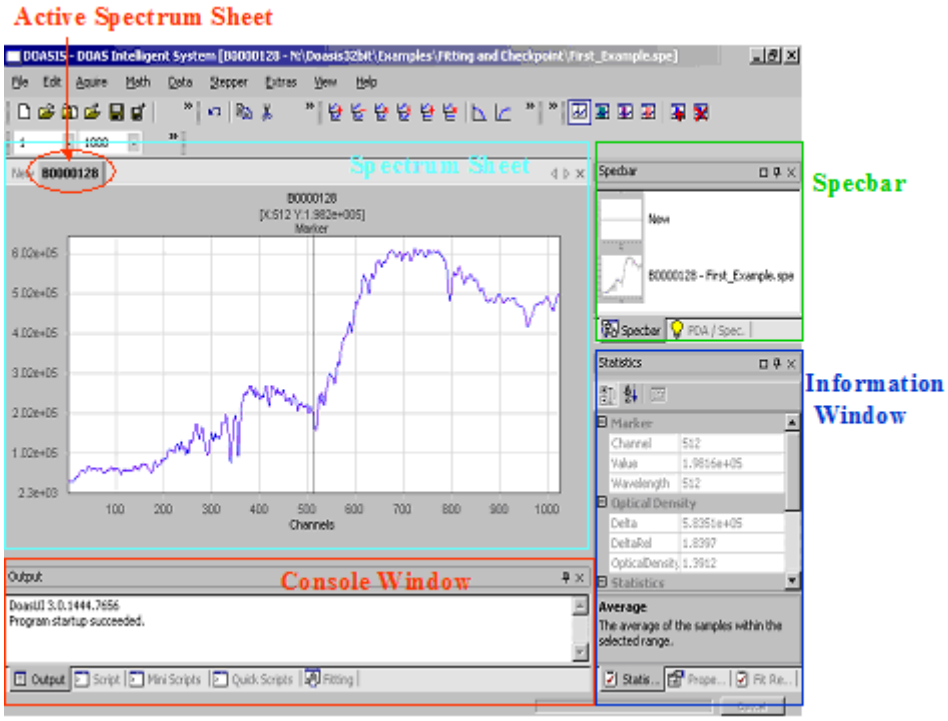

Figure 2.1: The main application window of the graphical user interface part *DoasUI*.

ferent script sheets are used for creating and editing automation scripts (automatic control of the program e.g. doing automatic measurements and data evaluation) and the fitting sheet for creating a fit scenario for spectra analyse.

2.3 Navigation in the active spectrum sheet

- *Mouse-Zoom*: Using the mouse is the easiest way to zoom. Click in the active spectrum sheet at the position of the new left margin. While holding down the left mouse key, drag the mouse towards the new right margin. A light grey rectangle opens to indicate the zoom area. Due to the auto-scaling of the vertical axis the height of the zoomed rectangle is irrelevant. The new limits become valid as soon as you release the left mouse key. This can be repeated as often as needed. To reverse the zoom by just one step drag the mouse from the lower right to the upper left while holding down the left mouse key. A pink rectangle opens, yet size and place don't matter, because it will zoom out according to the zoom in done before. To return to the un-zoomed state right-click anywhere in the graph. Any further right-click will toggle between the zoomed and un-zoomed state.

- *Numeric entry*: Select the properties sheet. There is a "ChartYAxis" entry among the subtitle marker & display. It is set on "auto" by default. When clicking on "auto" it can be changed to "fixed". If a numeric entry for the maximum and minimum values of the y–axis is favoured this can be implemented through an entry in the "ChartYAxisMax" and "ChartYAxisMin" boxes. In order to change the limits of the x–axis numeric values can be entered under "MaxChannel" and "MinChannel".

2.4 Limits: Setting markers and selecting ranges

During the evaluation of a DOAS spectrum it is frequently desirable to limit an operation to a range within the spectrum. For this purpose DOASIS provides four sets of markers: a fit–, math–, optical density– and general–purpose marker. To set and move markers several techniques can be used:
The markers can be activated under *view→markers→whichever marker you want*. When activated a coloured array will appear. Now you can either use the mouse to move, minimize or enlarge the array or you can use numerical entries, which you can set in the properties window under marker & display (for further information see 3.8). Another possibility, in case you don't like the coloured arrays, is to change these arrays to coloured lines (this might be especially useful if you want to overlay several markers). To do so choose *view→show marker range*.

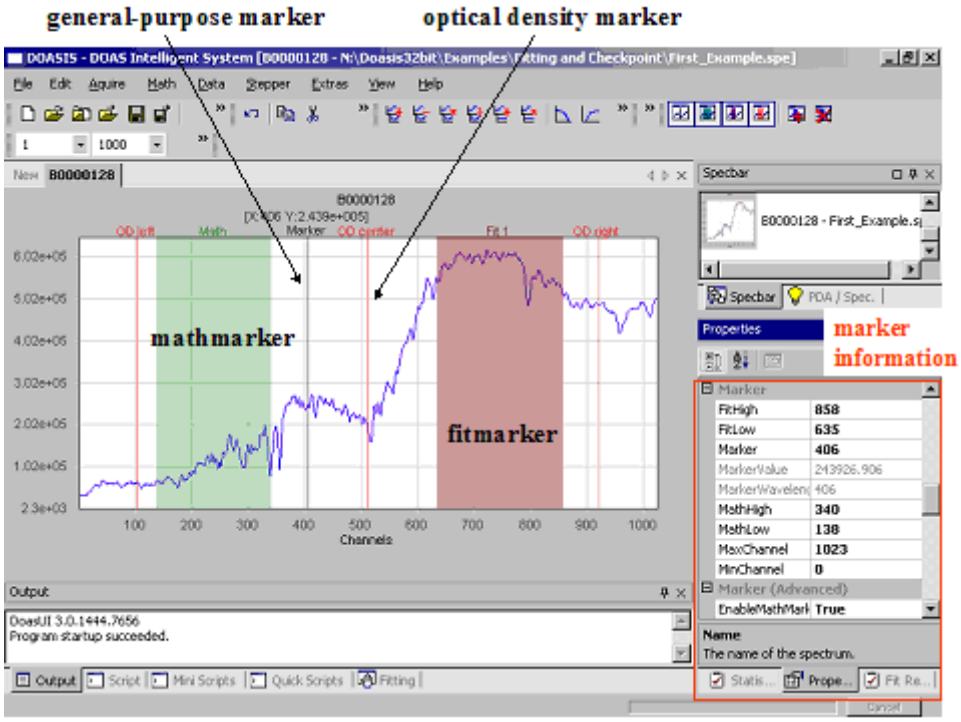

Figure 2.2: Example of the different kinds of markers.

2.5 Managing a collection of spectra

So far the focus has been on the active spectrum sheet, using just one spectrum. In DOAS work, usually a substantial number of spectra are involved, e.g. descendants of the raw spectrum as created by math operations, lamp, background and several reference spectra.
The central tool to manage a collection of spectra is the Spec bar. To get used to working with the Spec bar follow these steps:

- Open the demo spectrum from the spectra folder in the DOASIS program folder, 'First_Example.spe', if not already done so at the start of this tutorial, using the *file→open menu*.
- Open the spectra:

- 'BackgroundSpec.spe'
- 'DarkCurrentSpec.spe'
- 'HGRefSpec.spe'
- 'IO–Reference.sp2'
- 'Lamp–Reference.sp2'
- 'MeasSpec.sp2'
- 'NO2–Reference.sp2'
- 'OffsetSpec.spe'
- 'RohSpec.spe'

The active spectrum sheet displays the most recently loaded spectrum. In the Spec bar ten thumbnail pictograms of the loaded spectra are shown.
Each new spectrum is displayed on a new spectrum sheet. The spectrum sheets are sorted like a register. By clicking on the nametag, a spectrum will be displayed in the active spectrum sheet. A spectrum sheet can be closed by clicking on the x-button in the right top corner of the active spectrum sheet, yet this spectrum is still part of the current DOASIS session, because it is still displayed in the Spec bar.
The Spec bar is the main repository of all spectra that are or have been active during a DOASIS session. The pictograms represent the data of the spectra as stored in the PC memory. Whenever a new spectrum is created, loaded or duplicated, a new entry in the Spec bar is created.
A spectrum from the Spec bar can be displayed on a spectrum sheet at any time by clicking on the pictogram or on the spectrum's name.
To completely remove a spectrum from the DOASIS session, right-click on the pictogram or the name and choose "close". Note that by removing the spec bar icon, the entire spectrum sheet will be removed as well.

2.6 Oops: The undo–redo function

The interactive evaluation of spectra with the DOAS–method have elements of trial–and–error. You may want to experiment with various degrees of filtering, readjust windows for math operations, or compare the outcome of a previous operation with a current one. For this purpose, DOASIS offers an extensive, multi–level undo–redo concept.
Each operation, which modifies a spectrum, is preceded by an invisible backup of the initial state. Thus putting you in a position to undo/redo up to 6 times in a row, giving you the freedom to experiment extensively.
The undo–redo function is accessible through the Edit menu or the toolbar.

2.7 Some Maths

To prepare a spectrum (here: 'RohSpec.spe') for evaluation the following steps are needed (This example refers to active DOAS):

- Offset correction ('OffsetSpec.spe')
- Subtraction of the background light ('BackgroundSpec.spe')
- Removal of the spectral and trend features caused by the lamp ('Lamp–Reference.sp2')
- Extraction of the high frequency part of the spectrum, as it carries the differential absorption information.

While performing these steps, some basic mathematical tasks will be introduced.

- All spectra (background, lamp and roh) need to be offset corrected. To do so select 'BackgroundSpec.spe'. Then click on *math→correct offset*, choose 'OffsetSpec.spe' out of the list and press okay. Perform the same operations on 'Lamp–Reference.sp2' and 'RohSpec.spe'.

- Select the source spectrum: If not already displayed in the active spectrum sheet, click on 'RohSpec.spe' in the Spec bar.

- Create a duplicate: Create a copy of the spectrum (*Edit→Duplicate* or tool button), which will add a new pictogram to the Spec bar.

- Subtract background: Select the *math→spectrum operations→subtract spectrum* menu. A dialog appears requesting the name of the spectrum to be subtracted from our copy of 'RohSpec.spe' (make sure the copy is in the active spectrum sheet). The dialog lists all spectra that are held by the spec bar. Select 'BackgroundSpec.spe' and click 'Ok'. The spectrum graph will change only slightly, as the background intensity was only a few percent of 'RohSpec.spe'.

- Remove lamp spectrum: Select 'Lamp–Reference.sp2' from the *math→spectrum operations→divide spectrum* menu to divide the background–corrected 'RohSpec.spe'–spectrum by the lamp spectrum. The resulting spectrum already shows obvious absorption features, superimposed on a declining trend, which will be removed in the next step by high–pass filtering.

- High-pass filter: Select *math→high pass* or click the tool button. Change the number of iterations to '1000' and click ok. The trend has been removed, and absorption structures stand out clearly. There is still some noise that we will be removed in the next step.

- Smoothing: Select *math→low Pass* or click the tool button. Chose '5' as the number of iterations and click ok.

- Logarithm: Select *math→logarithm* or click the tool button.

- Save: Choose *file→save as* and select a location and a preferred name for your spectrum.

Chapter 3

The DOASIS Menu

This chapter will give you an overview of all the possible buttons and commands that you will find in your DOASIS Menu.

3.1 File

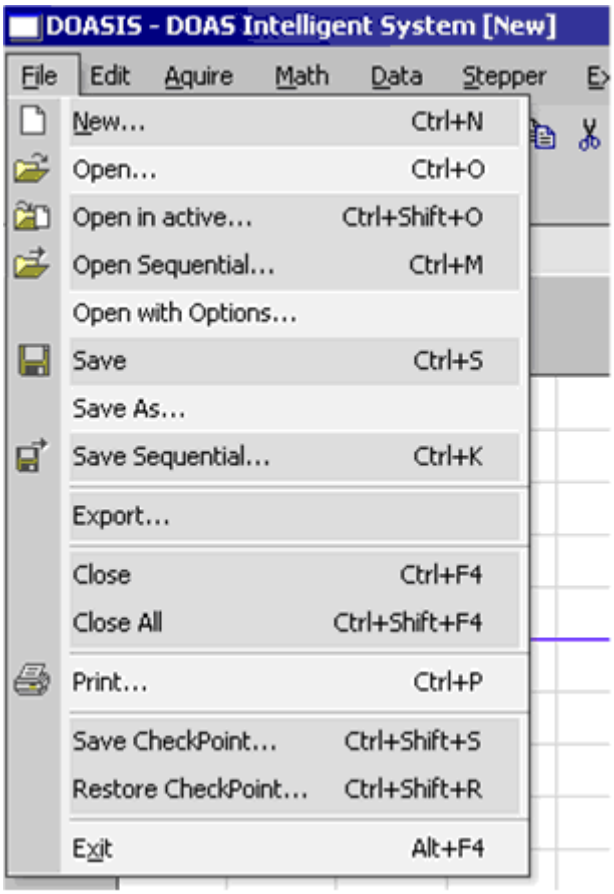

Figure 3.1: The file menu.

- To create a new spectrum, select the *new* command.

- If you want to open an existing spectrum from your file collection, choose *open*.
- *Open in active window* opens a spectrum file and replaces the current spectrum with the new one. Of course it will be opened either with the file or spectrum name according to what was chosen in the active window.
- It is possible to save the spectrum in the active spectrum sheet by using the *save* command. Note that the following file formats are possible:
  - .spe will save the spectrum with all properties
  - .mfc will save the spectrum with the most important properties
  - .std is the ascii version of mfc
  - .txt
  - .dat
  - .xs is a typical crossection file, which will save the wavelength information as an extra column.
- To open or save a whole sequential of spectra choose the *open sequential* or *save sequential* commands.
- You can save the spectrum in the active spectrum sheet under a different file name by using the *save as* command.
- There is a possibility to save your spectrum in the active window as an .emf file using the command *export*. If you do so you can reopen your spectrum later on with almost any graphic program.
- To close a spectrum in the active spectrum sheet simply use *close*.
- If you want to close not only the spectrum in the active spectrum sheet but also all the spectra that are currently open you can do so with the *closes all* command.
- Printing the spectrum in the active spectrum sheet is done by clicking on *print*. Here you can also decide if and which properties of your spectrum shall be printed with your spectrum by clicking on page set up.
- To save the current state of your session (including all spectra, the current layout, math. . .) for later use choose the *save checkPoint* command. To reopen this checkpoint use *restore checkPoint*.
- If you want to exit the application simply use the *exit* command.

3.2 Edit

- With the *undo* command you can restore the previous state. This can be done up to four times in a row.
- By using the *copy* command you can store an object temporarily in a buffer and than *paste* it into a place you desire. When copying a spectrum it is possible to choose whether to copy the whole spectrum data or only the currently selected row.
- The *cut* command is an extension of the copy command. It does not only copy the selected spectrum but deletes the old one when doing so. After that it can again be pasted into any chosen place.

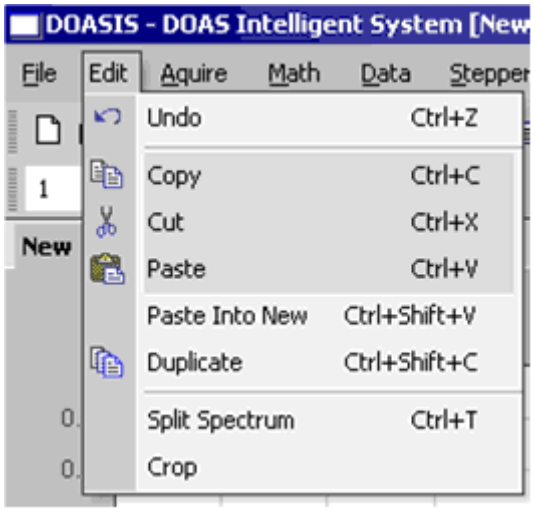

Figure 3.2: The Edit menu.

- If you want to simply paste a spectrum or part of it into a new window, copy the part you want and use the *paste into new* command. This will paste the copied part into a new spectrum sheet. This is a shortcut of the copy and past command since you don't have to open a new spectrum first.
- If you want to paste exactly the same spectrum as displayed in the active spectrum sheet into a new spectrum sheet simply use the command *duplicate*.
- To split a multidimensional spectrum into a set of one dimensional spectra where each spectrum is one data row of the multidimensional spectrum use the command *split spectrum*.
- To cut of part of your spectrum, select the part you want to get rid of and choose the command *crop*.

3.3 Acquire

- To start a scan with the previously set parameters (for example integration time and number of scans) you can use the *scan* command.
- The *dummy readout* starts a suitable high number of scans and minimum integration time. This is necessary to avoid the "memory effect" of photo diode arrays i.e. clearing residual structures of previous measurements. The resulting spectra are not displayed.
- To display the spectrograph controlling dialog use *PDA/spectrograph*. Further information on this window can be found in 6.4.
- *Auto scanning* will perform scans until a defined saturation is reached using the HMT serial controller.
- To get additional information about the ADC/DAC channels of the serial HMT Controller System parameters choose *system parameters*. A pop up window will appear in which the following entries can be viewed:
  - Temperature of the ambience
  - Temperature of the spectrograph

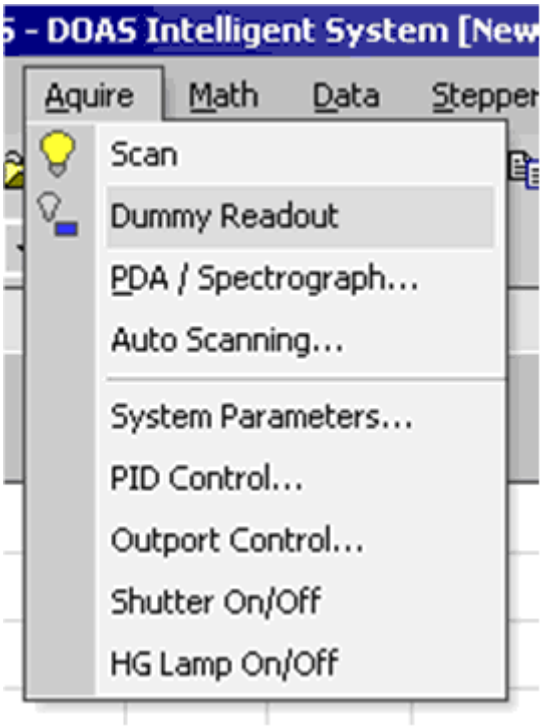

Figure 3.3: The Aquire menu.

  - Temperature of the PDA on the warm side of the peltier element
  - Temperature of the PDA on the cold side of the peltier element
  - Pt-1000
  - Pressure of the ambience

  All these parameters can be monitored over a period of time. To do so, activate the ones you want by setting a check mark into the little box right next to them, choose the intervals in which the results shall be displayed, how many times (defined through the number of log lines) you want them checked and then simply click on the start log button. Of course the logbook can be saved by using the save log button.

- *PDI* control
- With the *outport control* command you can control all 12V and 16V power supply outlets.
- The *shutter on/off* command will move a shutter in front of your CCD camera or back again.
- The mercury lamp which is used to calibrate spectra can be turned of or on by using the *HG lamp on/off* command.

3.4 Math

- ·If you choose the command *spectrum operations* you can *add, subtract, multiply* or *divide* the spectrum in the active spectrum sheet by a spectrum of your choice. When doing so note that the spectrum in your active spectrum sheet will be overwritten.

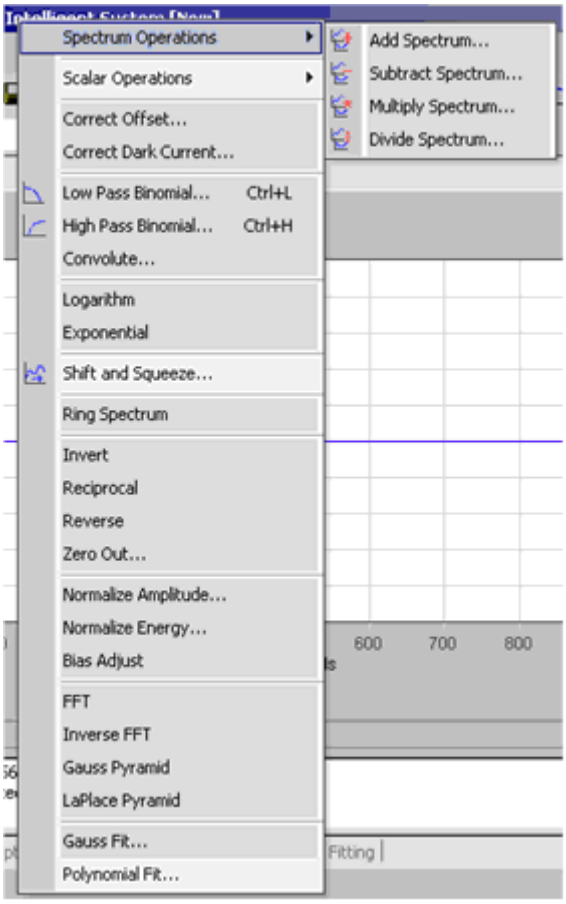

Figure 3.4: The Math menu.

- You can also *add, subtract, multiply* or *divide* a constant to the spectrum in the active spectrum sheet if you choose the command *scalar operations*. Again the spectrum in the active spectrum sheet will be overwritten.
- If you want to correct the offset of the spectrum in the active spectrum sheet you will find a *correct offset* command, which takes into account that you may have different iteration times and different numbers of scans. Just click onto the spectrum you want to correct, choose the correct offset command and insert your offset spectrum into the blank box.
- It is also possible to correct the *dark current* with the command located in the math bar using the same steps already described above.
- The *low pass binomial* command will perform a low pass binomial on the spectrum in your active spectrum sheet. The binomial filter uses the smallest binomial mask possible. This mask does the same as an averaging operation over three contiguous channels. Doing this will smooth out the spectrum, removing noise.
- The *high pass binomial* command will perform a high pass binomial on the spectrum in your active spectrum sheet. This means it will first do a low pass filter and will then divide your spectrum by the result of this low pass filter operation. This is very useful if you want to eliminate all your broadband structures.

- You can convolute a cross section with the instrumental function by using the *convolute* command.
- It is possible to take the *logarithm* or the *exponential* of the spectrum in the active spectrum sheet by using the corresponding commands.
- If you use the *shift* command you can shift the spectrum in the active spectrum sheet by as many channels or wavelengths as you fill into the blank box. The spectrum will be shifted to the right if you fill in positive numbers and vice versa. Note that if you shift your spectrum out of the diagram and than back into it, all the channels, which reappear, will be set to the value of the last one displayed.
- The *squeeze* command will squeeze the spectrum by the value, which you fill into the blank box.
- If you are using the sun as your light source you will have to correct the ring effect. You can do this by using the *ring spectrum* and *raman spectrum* commands.
- You can *invert*, take the *reciprocal* of a spectrum or *reverse* a spectrum by using the corresponding commands.
- By using the *zero out* command all the data of a spectrum below the limit, which you can fill into the pop up window, will be set to zero.
- If you choose the *normalize amplitude* command you can scale a spectrum in such a way, that the maximum value of the spectrum will correspond to a value of your choice. For example if you normalize the spectrum to 1 the spectrum will be multiplied by 1/(maximum value of the spectrum).
- The *normalize energy* command will normalize the surface area of the spectrum in the active spectrum sheet to the value that you fill into the menu of the pop up window. This is especially useful if you want to convolute as the convolution is not supposed to affect the order of magnitude of the spectral values. Considering this it is necessary to normalize the convolution core. In other words its area has to be one. Through this you can for example take the spectral line of a mercury lamp as a convolution core, normalize the surface area by using "normalize energy" to one and then convolute the line.
- Using the *bias adjust* command will subtract the mean value of a spectrum from itself.
- If you want to fourier transform the spectrum in the active window sheet just use the *FFT* command and if you want to do an inverse Fourier transformation use the *inverse FFT* command.
- The *gauss pyramid* is a set of low pass filtered spectra, which have been calculated out of the spectrum in the active spectrum sheet. In doing so each partial spectrum of the gauss pyramid only uses half of the frequencies of the previous spectrum. By doing so one achieves spectra of which the first one matches the original spectrum, the second one is smoothed in such a way that it only contains half of the frequencies of the original spectrum and so forth. Note that we are talking about frequencies of the Fourier transformation of the spectrum not the wavelengths.
- The *LaPlace pyramid* does in principal the same as the Gauss pyramid. The only difference is that the smoothed spectrum is subtracted from its preceding spectrum thus achieving a set of spectra where the first one only consists of high frequent parts of the spectrum and the last one only of low frequencies.
- Last but not least you can perform a Gauss fit on a spectrum by using the *Gauss fit* command.

3.5 Data

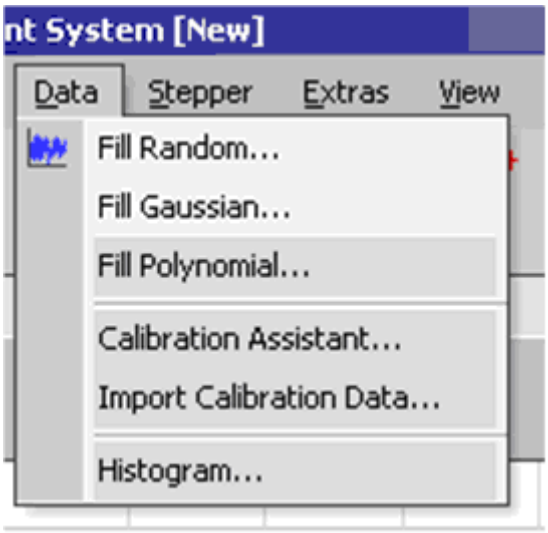

Figure 3.5: The Data menu.

- To fill the active spectrum sheet with random data use *fill random*. Use the number entry to define around which number you want to scatter.
- You can also fill the active spectrum sheet with a gauss curve. To do so choose *fill gaussian*. A window will appear in which you can set an x - value and a sigma.
- The third option is a polynomial. This is done by using *fill polynomial* after which a window will appear in which you can choose all the necessary parameters.
- To do a wavelength calibration of your spectrum the *calibration assistant* can be used. The calibration works as follows:
  - Scan an HG spectrum or any other kind of spectrum. The important issue is, that the wavelength of at least three or more features of the spectrum are known.
  - Place the marker in the middle of the feature/peak.
  - Enter the wavelength value of the marker's current position.
  - Press the *add* button.
  - Repeat the steps described above for all the known features. The more data points are available the better the result will be (but at least three wavelength positions are required to calculate the dispersion).
  - Press the *done* button.

  If the wavelength dispersion is calculated successfully, the result will be displayed on the current spectrum and the x–axis will be scaled in wavelengths rather than in channels. Note that the wavelength dispersion is determined using a polynomial of the order two.
- To find out more about *import calibration data* command see 7.
- The frequency distribution is given under the *histogram* command.

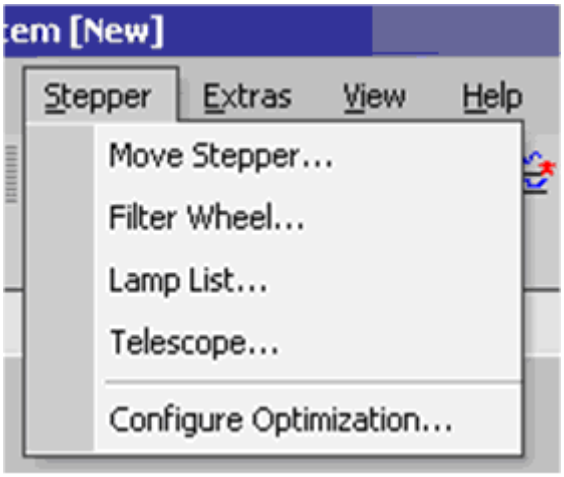

Figure 3.6: The Stepper menu.

3.6 Stepper

- If you choose the *move stepper* command a pop up window will appear. With this window you can control all your motors. For example if you choose teles_horizontal the motor number one will be activated (if you want to move your telescope in a horizontal direction it will have to be jumpered on the motor card as motor one otherwise what ever is jumpered as motor one will move) and so on. You can now decide how far the motor shall move. Note that there are two ways to do so: If you activate the move relative command the motor will move by as many steps as you tell him starting from the position it is already in. If this command is not activated the motor will move to the number you typed into the box meaning it will go to position (for example) 200. The current position is always displayed in the upper left of the window. By using the home button the motor will move to position zero. You can also set and save the start– and end – frequencies with which your motor shall be accelerated in this window.
- *Filter wheel*
- *Lamp list*
- *Telescope*
- *Configure optimization*

3.7 Extras

- *Dynamic data exchange* will open a communication protocol with which you can communicate with other programs.
- *Options*

3.8 View

Docking windows

- If you use the *reset workspace layout* command your workspace will be arranged, in particular the docking windows, according to the initial state.

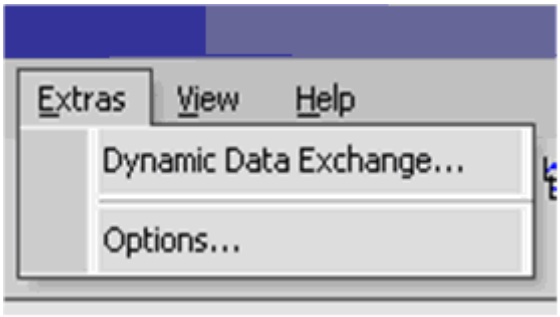

Figure 3.7: The Extras menu.

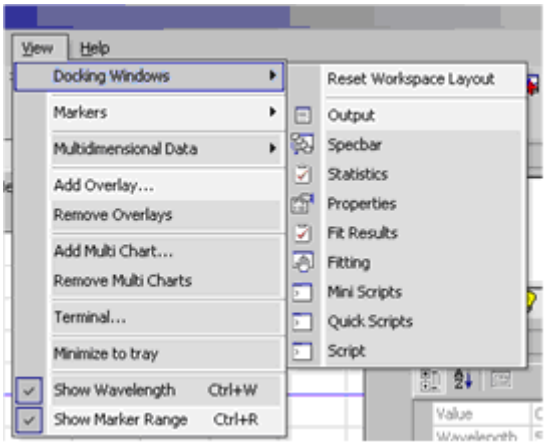

Figure 3.8: The View menu.

- The following commands will initialise docking windows in which different operations can be performed: *console, script, mini scripts, quick scripts* and *fitting*. For further information about how to use these docking windows please see 4.
- The commands *statistics, properties* and *fit result* will open a docking window in which you can find detailed information about your spectrum. Please also check 5.
- By choosing *specbar* a docking window will be initialised, in which you can manage your spectra collection.

Markers

- If you need a marker the *show marker* button will show or hide the marker in your active spectrum sheet.
- The *show math marker* command will create a coloured array, which you can move, minimize and enlarge, as you like. All mathematical operations you then wish to perform will only be applied to the coloured part of the spectrum.
- You can also choose to limit your fitting operations to a small part of your spectrum. To do so the *show fit marker* command will create a coloured array, which you can move, minimize and enlarge, as you like. Again all fitting operations you then wish to perform will only be applied to the coloured part of the spectrum.
- The show *OD marker* command makes it possible, to select a region of your spectrum in which the optical density shall be calculated.

- Apart from just defining one fit range with your fit marker it is possible to add an other fit range on top of the original one by using the *add fit range* command. This range will then be weighted double.
- To remove fit ranges the *remove fit ranges* command will remove all previously added fit ranges.

Multidimensional Data

- To select the first spectrum in a multidimensional spectrum use the *First row* command.
- To select the previous spectrum use *Previous row* and for the next spectrum use *Next row*.
- The *Last row* command will select the numRows-1 spectrum in a multidimensional spectrum.
- *row*

- If you want to overlay the spectrum in the active spectrum sheet by another spectrum, you can select the *add overlays* command. This will overlay the spectrum in the active spectrum sheet with a spectrum of your choice. You can choose between two options: Normal – this will simply overlay your spectra Fit all overlays – this will not only overlay your spectra but also fit them while doing so.
- The *remove overlays* command will simply remove previously added overlays from your active window.
- You might want to compare two or more spectra with each other without overlaying them. To do so just select the *add multi charts* command with which you can display the spectra next to each other.
- Of course you can remove previously added spectra with the *remove multi charts* command.
- When choosing the *terminal* command a window will open which will allow a direct communication via serial interface.
- If the *minimize to tray* command is enabled, the DOASIS window will vanish out of the taskbar when minimized and will appear as a small icon right next to the clock instead. From there it can be reopened through a double click.
- Through the *show wavelength* command you can determine if wavelength information shall be displayed or not, of course this will only apply to spectra which contain wavelength information in the first place (if you are not sure whether your spectrum contains this information or not, just check your spectrum properties under the entry "is wavelength valid").
- If you choose to display markers a coloured array will appear. Since it is sometimes more convenient to simply display coloured lines especially when overlaying marker ranges you can do so by activating *show marker range*.

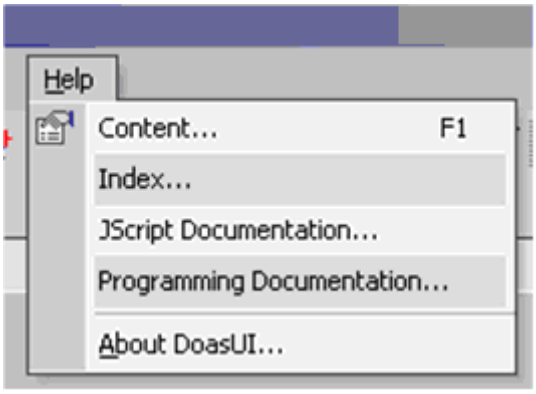

Figure 3.9: The Help menu.

3.9 Help

- If you choose the *content* command you will be shown an overview over the chapters and topics of the documentation.· Where as the index command will show an alphabetical order of the commands and topics used.
- To load the *Jscript documentation* or the *programming documentation* use the corresponding commands.
- *About DoasUI* will display who the credits for DOASIS go to.

3.10 Toolbars

For some of the menu entries a shortcut is available through the toolbars below the menu bar. The idea behind the toolbars is to make it easier for the user to do the same tasks over and over again. For example, if a menu function requires additional parameters you will be asked for them when you select the menu entry from the menu bar. To make the access to these functions faster, using the appropriate toolbar button executes the same action except the the user will not be asked for additional parameters again. Using the toolbar button will use the last function parameters unless they are invalid for some reason.
Here is a short example. If you choose the 'Subtract Spectrum' menu entry under the Math menu, you'll be asked for the spectrum that should be subtracted from the current one. The next time its enough to press the 'Subtract Spectrum' button from the math toolbar. This will automatically subract the spectrum selected the last time the menu entry was used. If the spectrum does no longer exist, you'll be asked to define a new operand again.

Chapter 4

The Console Window

In the console window you will find the Output, Script, Miniscript, Quickscript and also the important Fitting window. These windows are already available at the start–up of the DOASIS program. If you choose to close the console window you can restore the windows individually via the *view→docking windows* path.

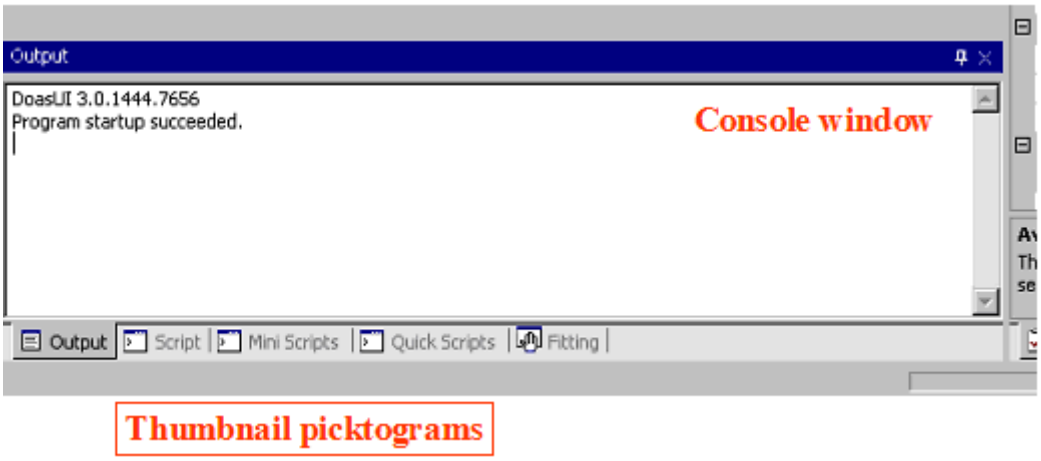

Figure 4.1: The Console window which has the Output tab selected.

4.1 Output

4.2 Script

The script dialog gives you access to the automation module for DOASIS. In the commando line you can enter the path of an existing Jscript or use the browse button. With the edit button the actual script will be opened for modification with an editor. You can set your preferred editor in *extras→options→jscript*.
With the start/stop/pause buttons the active script will be executed, stopped or paused. Be careful with the stop and pause buttons though: stopping requires a corresponding polling in your script (more in Jscript for dummies ? checkstop function). To pause means to suspend the execution of your script as well as the whole DOASIS program. When starting the script execution your script will be precompiled before it is executed. As default option script errors will appear in the console window. You can also choose the detailed error report

by choosing report full error information. (For further information about creating, handling and debugging Jscripts see – "Jscript for dummies", which will be coming soon!)

4.3 Miniscript

In the miniscript window you can easily type short scripts, which can be executed immediately. The most important functions for typical DOAS applications are already imported in the predefined header. More details and examples can be found in the J-Script for dummies documentation.

4.4 Quickscript

In the Quickscript window you can define short cuts for J-Script applications. Just choose one of the predefined short cuts from the list, double click on the line and a browsing window will open. Here you can choose a script application for your short cut. You can optionally define these short cuts system wide by activating this option in the header of the console window. This means, that even if the console menu or the Doasis program are inactive, the script, defined by the short cut, will be executed.

4.5 Fitting and Fitting Example

This chapter will explain, how to set up/create a fit scenario, execute a fit and store the results in a file for further use.

Restore checkpoint
To make things clearer please load the checkpoint fitting example via the *File→RestoreCheckpoint→Fit_Example.c*
path.
The example you have just opened is taken from measurements of an active–longpath DOAS set–up. It contains four spectra: The MeasSpec is the spectrum, which shall be evaluated. The other three spectra are reference spectra: The Lamp Reference – a spectrum, which contains the lamp structures. The Iodine–oxide and NO_2 reference spectra, which are used for the evaluation of the concentrations in the atmospheric spectrum (MeasSpec).
All these spectra have already been corrected – meaning, that offset and background corrections have been done for the Lamp reference and the MeasSpec and that the cross-sections of IO and NO2 have already been convoluted with the instrumental function.

Choose Fit-Range
The best way to start setting up a fit scenario is by choosing an expedient fit range. To do so it is useful to overlay the reference spectra with the atmospheric spectrum.
You will find the overlay–command under *view→add overlay.*
When you overlay the IO and the NO_2 reference spectra with the atmospheric spectrum choose the "fit all overlays" option – otherwise the y–axis will be scaled from zero to the maximum value of the spectra, which will not be helpful in this case.
Now you can easily choose a good fit range by using the *view→markers→show fit markers* path.
In our example we will choose a fit–range, which includes the three strongest bands of IO ($\sim$ 475 – 760). Simply place the fit markers in such a way, that these bands are within the colored range of your fit markers.

Fitting-options
In the console window you will find the fitting window. In the left part of this window is a

list in which you can enter the references that shall be fitted to your spectra.

> Please note: Doasis does not distinguish between cross sections and references. If you enter the cross sections of NO_2 and IO without any modification into this list - the fit coefficients will be negative. On the other hand the lamp reference is an absorption spectrum. The easiest way to avoid confusions is to invert your cross-sections before working with them.

To add a reference spectrum or a cross section to the list – you have to open the menu by double clicking on one line of the list. In the menu that opens you will again find a list of all spectra in the specbar.
Please choose the IO, NO_2 and Lamp reference for the fit–scenario.
For each reference of the list you can now choose the settings individually by clicking on the reference spectrum with the right mouse. This will open the fitting properties window, which consists of three parts. Since these three parts have a similar structure they will be explained conjointly:

Shift/Fit coefficient/Squeeze:

- The default parameter for each fit–option is normal – which means that there are no limitations or dependencies on the fit.
- You have the possibility to fix the resulting values (shift/squeeze/concentration) to a defined value.
- You can add limits to the fit parameters – e.g. exclude negative values for the concentration.
- You can also link the parameter to another reference – e.g. if the shift of IO shall be identical to the shift of NO_2 you can link the shift of the IO reference spectrum to the NO_2 reference spectrum.

In our example, to make things a little easier, we will stick to the default values. Do feel free though to try out some of the options as you move along.

Polynomial degree
In the centre of the fitting window you can choose different polynomial degrees – detailed information on the resulting polynomial will appear in the list after the fit procedure. Information about the Chi–Square and the Fitsteps will also be shown in this part of the window after the fit procedure.

More fitting properties
There are five buttons on the right side:

- The first button will execute the fit scenario that you have configured in the chosen fit–ranges with the spectrum in the active spectrum sheet.
- The second button allows you to save the actual fit scenario into a file with a name of your choice.
- With the third button you can load an existing fit scenario.
- The fourth button contains additional fitting properties:
  You can optionally decide to take the logarithm of the spectra automatically before the fit is executed (another possibility is to do this by pre–processing your spectra with a J–script).
  Further more you can limit the fit iteration steps to a maximum value. For additional information on the evaluated spectra look at the entries made in the spectrum

properties. You can choose from a list which entries shall be stored together with the fit–results in an ascii-file. The name of the file can be selected freely.
You can decide if you want to have additional header lines incuded at the top the fit result file. These lines include information about the DOASIS version used, the date and time of creation and the current fit scenario file name. The user can also add his/her own comment to be inluded.

- To save these values (including additional information from the spectrum properties) to an ascii-file use the fifth button.

Execute Fit-scenario
To execute the scenario please click the first button with the exclamation mark. The fit results of the reference spectra on the list, the polynomial and the residuum will appear in a multi-chart view sheet for supervision.
In the multi-chart view, the reference spectra multiplied with the fit coefficient are overlaid with themselves with an added residual. Additionally the calculated result–spectrum on the multi–chart will also be available in a single sheet in the taskbar and in the specbar.
You now have the option to save single spectra or to print them (see menu entry *file→print→multi-chart*).
All calculated parameters, like the fit coefficient, the shift and squeeze results and the iteration steps of the scenario appear in the fitting window.
You can now save these values into an ascii–file with the fifth button.

Chapter 5

The Information Window

This chapter will give you a short overview over the features that can be found in the information window. You will find that it is divided into three separate windows: The Statistics, Properties and Fit Results window.

5.1 Statistics

Marker

- Here you can find information about your marker. You can see which *channel* or *wavelength* the marker is placed on and also which *value* on the y–axis this corresponds to

Optical density

- *Delta*
- *DeltaRel*
- The value of your optical density is given in the *opticalDensity* box.

Statistics

- All the math info can be found here: The *average* gives you the average value of your spectrum, the *deviation* and *variance* of your spectrum can also be found here. Another important figure is given in the *max* and *min* lines: These tell you what maximal and minimal values your spectrum has.

5.2 Properties

Information
In this window you will find important information about your spectrum such as:

- The *centerWavelength* is only given for backwards compatibility, all users who work with DOASIS for the first time should simply ignore this entry.
- Which *elevationAngle* you where at.
- How long your *exposureTime* was.
- The *name* of your spectrum.

- How many scans where made (*numScans*)
- What the *startDate* was.
- What the *startTime* was.

Information Details
Further information that might be needed will be given in this section:

- Which *altitude* you where at.
- Who the *author* was.
- At what *azimuthAngle* you where.
- Which *device* was used.
- *flags*
- *gain*
- At what *latitude* the scan was made.
- How long the *lightPath* was.
- What kind of *lightSource* was used – meaning what kind of lamp or maybe the sun.
- At what *longitude* the scan was made.
- Whether this is the original spectrum or if it has already been *modified*.
- *multiChannelCounter*
- *objectKey*
- What the *pressure* of your ambience was.
- Any *remark* can be added here.
- *scanMax*
- What the *site* was called
- At what time the scan was stopped (*stopTime*)
- What the *temperatureAmbient* was.
- The *wavelengthLinearDispersion* is only given for backwards compatibility, all users who work with DOASIS for the first time should simply ignore this entry.

Marker

- The entries *fitHigh* and *fitLow* will show you the exact channel or wavelength your fit marker is located on.
- You can find the position of your marker given either in channels (*marker*) or wavelengths (*markerWavelength*) as well as its corresponding position on the y–axis (*markerValue*).
- You can find the exact location of your math marker by checking the *mathHigh* and *mathLow* entries.

- In order to set a maximum or minimum value for your x–axis, enter the numeric values in the boxes *maxChannel* or *minChannel*

Marker (Advanced)

- If the *enableMathMarker* is set to true any mathematical operation is limited to the data selected by the math range. Otherwise always the whole spectrum will be affected.
- The position of the optical density marker is given by three different entries: The centre is given by the *opticalDensityCenter* entry, the left by the *opticalDensityLeft* entry and the right by the *opticalDensityRight* entry.

Spectral data

- The *calibPolynomial* gives you the used polynomial for your dispersion equation.
- If *isWavelengthValid* is set to true the data array listed under the wavelength–property contains valid channel–to–wavelength information. Otherwise the data array contains only channel numbers.
- The number of channels used is dependent on whether you measured with a PDA or CCD array and is given under *Nchannel*.
- *NumRows*
- *Rows*
- *SelectedRow*
- *SelectedRowIndex*
- *Wavelength*

Statistics

- You can see the *average* of your spectrum in this box.
- The peak-to-peak distance is given in the *delta* box.
- Under *deltaRel* you will find the root mean squared of your delta.
- The maximum and minimum values of you spectra are given in the *max* and *min boxes*.

Statistics Details

- *deviation*
- Of course you can find the *opticalDensity* and its *variance* in the corresponding boxes.

View

- The title of the x–axis is given by *ChartXAxisLabel*
- Your y-axis is charted automatically by default to change this setting, double click on *chartYAxis* and it will be set to fixed.
- The title of the y–axis is given by *ChartYAxisLabel*

- If you want to set a maximum or minimum value for your y-axis you can do so by making an entry under *chartYAxisMax* or *chartYAxisMin*.
- The *overlayMode* entry is set to normal by default and can be changed to rescaleOverlay by double clicking on it.

5.3 Fit Results

- *coefficient*
- coefficientDefault
- *Shift* gives you the calculated shift of your spectrum. That you need to shift the reference spectrum might be necessary if for example the temperature of your measured spectrum isn't the same as the temperature of the reference spectrum.
- *ShiftDefault* contains the initial value of the fit.
- The error of your shift is given under *shiftError*.
- How far your reference spectrum was stretched or squeezed is given under *squeeze*. The reason why it is necessary to do so might be that a PDA structure needed to be corrected.
- *SqueezeDefault* contains the initial value of the fit.
- Again, the error of your squeeze can be found under *squeezeError*

Chapter 6

Controlling Hardware With DOASIS

6.1 Instruments that can be controlled by DOASIS

- Acton
- HMT AutoScan
- HMT Fixed Grating
- HMT USB MicroStepper
- HMT USB MultiStepper
- Mini DOAS
- Jobin Yvon using a serial HMT controller
- Ocean Optics:
  - ADC 1000
  - USB 2000
  - USB 2000+
  - USB 4000
  - HR 2000
  - HR 4000
  - QE 65000
- Slotted Disc Machine
- Triax

6.2 How to connect an Ocean Optics spectrograph to a measurement PC

This section covers how to properly install the Ocean Optics drivers on a measurement PC and how to connect a new Ocean Optics spectrograph to this PC.
As an example, the USB 2000 is used, but it could be any other Ocean Optics spectrograph supported by DOASIS (see 6.1).

Ocean Optics software can be downloaded from here:
http://www.oceanoptics.com/technical/softwaredownloads.asp

1. Install Ocean Optics OOIWinIP (version 4.0.11.6 or newer).
2. Install Ocean Optics OOIBase32 (version 2.0.6.5 or newer).
3. Connect the USB 2000 to the USB port of your PC. If you connected it before step 1, then Windows may have installed some wrong drivers by itself. In that case, plug the USB 2000 out, uninstall its driver, follow steps 1 and 2 and then plug it in again.
4. Windows informs you to have found a new device. In the first dialogue, decline to connect to the Windows Update. In the second one, let the software be installed automatically. You should now get a message saying that the USB 2000 was installed properly.
5. Start OOIBase32, select the USB 2000 and make sure that it works, i.e. that it reads out the spectra and displays them on the screen.
6. Close OOIBase32.
7. Start DOASIS, in the field "device" select the USB 2000 and see, if its serial number shows up. If the serial number does not show up, close DOASIS, start once again OOIBase32, let it display the spectra of the USB 2000 again and close it.
8. Now, DOASIS should display the serial number of the USB 2000. If so, then it has recognized it and from now on, you won't need the step of initialization using OOIBase32 anymore.

Note: Please keep in mind of not having OOIBase32 and DOASIS running at the same time. Both will try to access the spectrograph and may slow each other down or block completely each others access to the hardware.

6.3 How to operate two Ocean Optics spectrographs with DOASIS at the same time

The driver of Ocean Optics does not support the usage of more than one spectrograph at the same time. Thus, DOASIS has been programmed to handle more than one spectrograph anyway.
To operate two Ocean Optics spectrographs at the same time, one also needs two instances of DOASIS running simultaneously. In detail, please follow these steps:

1. Connect both spectrographs to your PC. Make sure, that their drivers are installed correctly (therefore, see 6.3).
2. Start OOIBase32 and choose one of the spectrographs, called "spectrograph 1" in the following.
3. Close OOIBase32 and start the first instance of DOASIS.
4. In this instance of DOASIS, you should be able to operate the spectrograph 1 as usual.
5. Open the second instance of DOASIS. In the field "device", select the other spectrograph, called "spectrograph 2" in the following. You should be able to choose the spectrograph, but not to alter the diplayed serial number in the field "USBSerial". This one probably still shows the serial number of the "spectrogrph 1".

6. Close the second instance of DOASIS. At the moment, you have only one (the first one) instance of DOASIS open. Now, start again a second instance of DOASIS.

7. In this second instance, the field "device" should already show the correct type of the "spectrograph 2". But now, you should also be able to overwrite the "USBSerial" with the correct serial number of the "spectrograph 2". Please do so.

8. Now, you can use both Ocean Optics spectrographs, each one with its own instance of DOASIS, at the same time.

Note:

- After closing both instances of DOASIS or after rebooting the PC, please start again with the second item.

- For how to operate two Ocean Optics spectrographs with two different JScripts, please see in the **JScript Tutorial** the chapter "How to operate two Ocean Optics spectrographs with two JScripts at the same time".

6.4 Examples

Example Acton/Longpath
An example for setting up measurements of a typical Hoffmann/Acton combination is given here:
It is required, that you correctly connect one COM port of your PC to the Hoffmann controller with a serial cable. In the menu: *acquire→PDA spectrograph* a dialogue opens, where you have to enter all required settings for your system.
First you choose the spectrograph type as the correct device (in the top of the window) – in our case this will be the Acton. In the HMT serial communication the following settings are suitable:
The baud rate is 57600kB. In the port HMT menu point you have to enter the correct port of communication. In *test communication* you can choose the option: test communication, which will give you the information if DOASIS found the correct hardware on the given port. Additionally in the console window a message appears if the initialisation succeeded or failed. After a successful initialisation of the new device you can start your measurements:

In the device settings you can choose the grating and the wavelength for your measurement, whereas you can choose the exposure time and scan number in the *scan settings*:

- *Scan*: This button will start the scan with the chosen settings.

- *Initialise* is still not properly working – but should check the serial communication with the HMT controller.

- *Device* will open a window where all scan settings are more clearly arranged.

- *Dummy readout*: This button is used to clear the PDA from remaining structures of previous measurements. This is realised by reading out the PDA with a suitable high number of scans and minimum integration time. The resulting spectrum is not displayed.

Example Ocean Optics/scattered light
To work with Ocean Optics you will have to install Hoffmann USB Aktive X Control Software and Ocean Optics and you need to connect the instrument to the USB.
At first you have to start Ocean Optics and choose *connecting to the first available USB2000*, the program should then find the right serial number. If not select the right serial number and have a look at the displayed spectrum. Now, when you start Doasis a window called

configure hardware appears, in which you can choose the Spectrograph Type and several other settings. After you have selected the appropriate settings click "ok" and Doasis will open.
Use *aquire→PIDControl* to open a new window where you can set the desired temperature of your spectrograph by entering it into the provided field.
Wait until the actual temperature is constant and in the range you want to have before proceeding.
Use *aquire→PDA/Spectrograph* to open the PDA/Spec-Window. Under device you can choose the Ocean Optics USB 2000 and under scan settings you can set exposuretime [msec] and the number of scans (note that the lowest exposuretime your Ocean Optics can handle is 3msec). Choosing the command *scan* will now start a scan.

Chapter 7

Advanced Topics

This chapter will describe some of the more complex functions of Doasis like wavelength calibration and reference spectra preparation.

7.1 Wavelength Calibration

Doasis allows the definition of a channel-to-wavelength calibration polynomial. This polynomial can be defined for each spectrum separatly thus each spectrum can have a different wavelength scale. Additionally the calibration polynomial can be set as default for new spectrum object as well as be used by the spectrograph devices as their default calibration. To define the calibration polynomial you can choose the manual way by defining the calibration polynomial coefficients using the properties windows of the spectrum or you can use the Calibration Assistant to determine the calibration polynomial using a least squares fit. To use the Calibration Assistant do the following:

1. Record a spectrum where you know the wavelength of at least 3 features within the spectrum eg. a HG-spectrum.
2. Start the Calibration Assistant from the Data menu.
3. Press 'Next'.
4. Place the Marker on one of the known spectrum features.
5. Press the 'Get Marker' button in the Calibration Assistant. The current marker position should appear in the text box left to the button.
6. Enter the wavelength of the feature in the next textbox and press the 'Add' button. The channel-wavelength data point will be added to the list on the left side.
7. Repeat step 4. at least two times. Its necessary to define at least 3 different channel-wavelength data point. The more data points given, the more acurate the calibration result will be.
8. Once you've defined enought data points press 'Next'.
9. Define the order of the resulting polynomial. Normally it should be sufficient to use a polynomial of order three or less.
10. Press 'Next'
11. If the polynomial fit was successful, you should now see a plot of the determined polynomial. To change the polynomial use the Back-buttons. Otherwise press 'Next'

12. Now you need to define where the polynomial should be used. You have the following options:

    - *Current Spectrum* The polynomial will be used in the current spectrum.
    - *All open spectra* The polynomial will be used in every spectrum listed in the Specbar.
    - *Default for new spectra* The polynomial will be used as default calibration polynomial for new spectra.
    - *Current spectrograph* The polynomial will be used by the currently selected spectrograph. Any spectrum recorded with this device will then get the spectrograph's wavelength calibration.

13. Press 'Next' and 'Finish'. That's it!

Howevery you can always remove the wavelength calibration by deleting the polynomial's coefficients of if you set the 'IsWavelengthValid' property to *false*.

7.2 Convolution and Downsampling

To use a high resolution reference spectrum with you measured data, its necessary to prepare the reference spectrum in a way that the aperture function of your spectrograph will be simulated. A good approximation for the aperture function is to record a very sharp peak with your spectrograph and than convolute the reference spectrum with the recorded peak and downsample the spectrum to the wavelength calibration of the spectrograph. The convolution can be done in Doasis very easily although the convolution tool does a general convolution using a given kernel function.

1. Prepare a spectrum that represents the convolution kernel. Eg. record a HG spectrum.
2. Please the Math Marker around the convolution kernel. (Select one of the peaks in the HG-spectrum).
3. Place the Marker on the center of the convolution kernel. (Set the maker right in the middle of the HG-peak). You can also use the 'Auto search kernel center' feature in the convolution dialog. In this case its not necessary to place the marker manually.
4. If the convolution result needs to be resampled to another wavelength range, create a spectrum that is calibrated to the desired wavelength range.
5. Open high resolution reference spectrum and make it the visible one.
6. Select 'Convolute' from the Math menu.
7. Select the spectrum that represent the convolution kernel.
8. Select either the spectrum that holds the target wavelength information or the reference spectrum. If you select another spectrum as convolution target than the reference spectrum itself, the convoluted spectrum will be resampled to the wavelength range defined in the target spectrum. Otherwise just an inplace convolution on the reference spectrum will be done.
9. If you want the convolution to find automatically the center of the convolution kernel, check the 'Auto search kernel center' checkbox. If enabled, the convolution will assume that the maximum value inside the math limits represents the center of your convolution kernel.
10. Select on of the convolution kernel options:

- *Normal convolution kernel* Use this option if the convolution kernel should be used as it is. No rescaling or anything else will be applied to the kernel.
- *Normalize convolution kernel* In this case the convolution kernel will be normalized like defined in equation 7.1. This option should be used when a reference sectrum will be prepared with a HG-peak, since the normalization will ensure that the scale of the reference spectrum will stay the same and only a smoothing operation will be applied.

  The normalized kernel $k(x)$ of a given convolution kernel $s(x)$ with the given math range $l \ldots h$ is given by the following equation:

$$k(x) = \frac{s(x) - s_{min}}{\int_l^h s(x) - s_{min} dx} \tag{7.1}$$

$$s_{min} = \min s(x) | l \leq x \leq h \tag{7.2}$$

11. Press 'OK' to start the convolution.

Note: If one of the three spectra required for convolution does not contain a valid wavelength calibration, the convolution will work on channel basis. Therefore the downsampling to the target wavelength will result in a simple resampling of the whole reference spectrum to the number of channels of the target spectrum.

7.3 Fitting

Essential for a DOAS analysis is the non linear fitting. Doasis makes fitting quite easy using the Fitting tool in the console window. A simple fit can be done doing the following steps:

1. Prepare your measurement spectrum and reference spectrum.
   Note: If one of the spectra used for fitting does **not** contain a valid wavelength calibration, the fit will operate on channel basis!
2. Select your measurement spectrum and define the desired fit ranges.
3. Select the fit window.
4. Select the reference spectra used for fitting by clicking on the first column on one of the lines of the list box. Select the reference from the drop-down list.
5. Define special parameter setting for each reference by double-clicking on the a reference entry or using the button at the end of the line. The current fit implementation allows to:
   - Define a different start value for a parameter.
   - Fix any parameter to a defined value.
   - Limit any parameter to a given range. If 'hard limit' is used, the fit will ignore all results where a parameter is outside the valid range. Using soft limits still allows invalid parameter values, but the result gets a penalty that increases exponentially the more the parameter is outside the valid bounds.
   - Link any parameter to another spectrum.
6. Open the fit properties dialog.
7. Define whether the measurement spectrum should be logarithmed by the fit or if its already in logarithm space.

8. Select the spectrum properties that should be store in a result file as well.
9. Select the desired fit model and define the additional model parameters.
10. Define the fit range. If you press the 'Get from current spectrum'-button, the fit ranges of the current spectrum will be used.
11. Close the properties dialog.

You can now start fitting or first save the complete fit settings into a scenario file. The next time you want to use the fit settings, its enough to open the fit scenario file. All required information as well as all reference spectral will be loaded than from the scenario file.
If you set any polynomial order to less than zero (< 0) the polynomial will not be used during the fit. Currently its possible to add two polynomials: The usual DOAS polynomial and an additional offset polynomial.
It you choose to use the DOAS fitting model, the well known DOAS equation is used as model function for the fit. Starting from the DOAS equation given by:

$$I(\lambda) = e^{\sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda)} + O(\lambda) \tag{7.3}$$
$$\tag{7.4}$$

we transform everything into logarithm space to get at least some linear parameters.

$$\ln(I(\lambda) - O(\lambda)) = \sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda) \tag{7.5}$$
$$\ln\left(I(\lambda)\left(1 - \frac{O(\lambda)}{I(\lambda)}\right)\right) = \sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda) \tag{7.6}$$
$$\ln(I(\lambda)) + \ln\left(1 - \frac{O(\lambda)}{I(\lambda)}\right) = \sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda) \tag{7.7}$$

For very small $\frac{O(\lambda)}{I(\lambda)}$ we get

$$\ln\left(1 - \frac{O(\lambda)}{I(\lambda)}\right) \approx -\frac{O(\lambda)}{I(\lambda)} \tag{7.8}$$

and we can use

$$\ln(I(\lambda)) = \sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda) + \frac{O(\lambda)}{I(\lambda)} \tag{7.9}$$

for DOAS fitting, where $I(\lambda)$ is the already high pass filtered measured spectrum. c_i is the fit coefficient, s_i the shift and t_i the squeeze value of the reference spectrum $\sigma_i(\lambda)$. $P(\lambda)$ denotes the DOAS polynomial and $O(\lambda)$ the additional offset polynomial. Although the offset polynomial $O(\lambda)$ is not exactly correctly represented in this case. But the results are nummerically more stable and therefore this method should be the prefered one to evaluate the data.
Selecting the intensity fitting model, the evaluation is done in intensity space. The intensity fitting model evaluates $O(\lambda)$ correctly by using the following equation:

$$I(\lambda) = e^{\sum c_i \sigma_i (s_i + t_i \lambda) + P(\lambda)} + O(\lambda) \tag{7.10}$$

If the fit was successful, you should see a result overview to visually ensure the result if correct. The exact results of the different species will be display in the fit window. Using the 'Append to Result File'-button stores the fit results in the selected ASCII file.

Note: If all reference spectra and the measurement spectrum have a valid wavelength calibration, the fit automatically operates in wavelength based mode. Thus any parameters are now given in wavelength units! This includes any parameter limits or fixed values defined in the fit scenario!
If at least one spectrum is missing a valid wavelength information, the fit works in channel based mode and all parameters are given in channels then.

Chapter 8

Glossary

In this section the commands avaiable in DOASIS will be described in greater Detail. Since most commands are also available in JScript, the syntax will also be explained.

8.1 Math Menu

All math operations are applied to the range that is marked by the math marker, which is the selection highlighted with a green colour.

8.1.1 Scalar Operations

The scalar operations are applied to the current spectrum sheet. The current spectrum will be overwritten by the new spectrum. Since in both intensity spectra and optical density spectra the y-axis values are realized as of data type double, one can add/substract/multiply/divide a constant to the spectrum by specifying this constant in the popup window. You can use both decimal or exponential notation, e.g. $4.25e-05$ instead of 0.0000425. For each scalar operation, the popup window will remember the last number to make it easier to apply the same scalar operation to different spectra.

Warning: ***Division by zero*** *causes no error, but sets the value to zero. Therefore, if a spectrum is divided by zero, the intensity is set to zero everywhere.*

JScript Syntax: Some examples with the constant 2.5 applied to the current spectrum sheet:

```
SpecMath.Add(Specbar.CurrentSpectrum,2.5);
SpecMath.Sub(Specbar.CurrentSpectrum,2.5);
SpecMath.Mul(Specbar.CurrentSpectrum,2.5);
SpecMath.Div(Specbar.CurrentSpectrum,2.5);
```

8.1.2 Spectrum Operations

Spectrum operations are such as channelwise addition, subtraction, multiplication. In contrast to the scalar operations, the current spectrum is not modified by a constant, but each

channel is modified by the value of the same channel in the reference spectrum, which has to be specified in the dialog box.
Notice that spectrum operations require that both current spectrum and reference spectrum have the same range of channels/wavelengths. If this is not so, an error may occur.
There are three modes how to modify the current spectrum by spectrum operations:

- **normal: the values of a certain channel are added/subtracted.**
- **scan weighted: before addition/subtraction/..., the reference spectrum is muliplied by an overall factor, namely the ratio $NumScans_{specCur}/NumScans_{specRef}$. This command is for example useful to reduce scan-dependen effects (like offset correction).**
- **time weighted: before addition/subtraction/..., the reference spectrum is muliplied by an overall factor, namely the ratio $\frac{NumScans_{specCur}*ExposureTime_{specCur}}{NumScans_{specRef}*ExposureTime_{specCur}}$, which is the ration of the overall scan times ($t_{overall} = NumScans * t_{exposure}$) This command is for example useful to reduce time-dependend effects (like dark current correction).**

JScript Syntax: For example, if the Specbar contains a spectrum named "RefSpec", a scan-weighted addition is done by

```
SpecMath.Add(Specbar.CurrentSpectrum,Specbar.Spectra["RefSpec"],
SpectrumOperandMode.ScanWeighted);
```

For time-weighted spectrum operations, the flag `SpectrumOperandMode.TimeWeighted` has to be used instead. For normal mode, the third argument can be omitted.

8.1.3 Logarithm

The logarithm command takes the logarithm $log(y)$ (to the basis e) of the value y of each channel in the math range.

Warning: *Taking the logarithm of a* ***nonpositive number*** *produces no error. Instead, the value is set to zero. This causes a spectrum that was "continuous" before to become* ***uncontinuous*** *in the logarithmic graph since the difference between* $\log(0.001) = -6.91$ *and* $\log(-0.001) = 0$ *is much larger then it was before. Please ensure that your spectrum has no negative values to avoid this.*

JScript Syntax: Taking the logarithm of the current spectrum is done by:

```
SpecMath.Log(Specbar.CurrentSpectrum);
```

8.1.4 Exponential

The exponential command takes the exponential $exp(y)$ of the value y of each channel in the math range.

JScript Syntax: Taking the exponential of the current spectrum is done by:

```
SpecMath.Exp(Specbar.CurrentSpectrum);
```

8.1.5 Shift and Squeeze

Shift and Squeeze are sometimes used to calibrate a measured spectrum. The usual way to do this is to use the Calibration Assistant which determines a channel-to-wavelength polynomial. But sometimes only a certain range shall be modified. The commands work on channel basis, not on wavelength basis. In fit routines, shift and squeeze parameters also play a great role, since reference spectra might differ slightly in their scaling from the measurement spectrum.

The shift command shifts the spectrum to the left for postivie values and to the right for negative values. The spectrum is shifted as many channels as is entered in the dialog box. You can enter decimal numbers, but in the end only are rounded to integers.

The sqeeze command squeezes a region into the math region, i.e. for a squeeze number $s > 1$ the range which is s times wider than the math region is mapped into the math region by dividing the channel numbers by s. The fix point of the squeeze operation is the lowest channel of the math range (left border). For values $s < 1$ the range is actually not squeezed, but stretched. $s = 1$ is the identity.
In a shift and squeeeze, a range (partially) outside the math range is shifted/squeezed **into** the math range. The math range is **not** shifted/stretched in a region (partially) outside the math range. Therefore, **only values within the math range will be altered.**

Warning: *If the region that shall be mapped into the math range is outside the full range of the spectrum (for example if the whole spectrum is marked and shall be squeezed), the range within the math range for which no values are available are all set to the value the lowest/highest channel (the right/left border of the spectrum).*

JScript Syntax: Shift and Squeeze can be done by:

```
SpecMath.ShiftAndSqueeze(Specbar.CurrentSpectrum, fShift,
fSqueze);
```

where `fShift` and `fSqueeze` are float variables or numbers. Alternatively, there are seperate commands for both shift and squeeze:

```
SpecMath.Shift(Specbar.CurrentSpectrum, fShift);
SpecMath.Squeeze(Specbar.CurrentSpectrum, fSqueze);
```

8.1.6 Invert

The invert command takes the negative $-y$ of the value y of each channel in the math range.

JScript Syntax: Inverting the spectrum is done by:

```
SpecMath.Invert(Specbar.CurrentSpectrum);
```

8.1.7 Reciprocal

The reciprocal command takes the reciprocal $1/y$) of the value y of each channel in the math range.

Warning: ***Division by zero*** *causes no error, but sets the value to zero. Unfortuntaely this causes incontinuities in spectra that have zero points. So be aware of this fact!*

JScript Syntax: Taking the reciprocal of the current spectrum is done by:

```
SpecMath.Reciprocal(Specbar.CurrentSpectrum);
```

8.1.8 Reverse

The reverse command reverses the order of channels within the math range, i.e. the first channel in the range becomes the last (and vice versa), the second becomes next to last and so forth.

JScript Syntax: Taking the reverse of the current spectrum is done by:

```
SpecMath.Reverse(Specbar.CurrentSpectrum)
```

8.1.9 Zero Out

This command sets all those values of the channels within a marked range to zero, which absolute value is below the value that is specified in the dialog box.

JScript Syntax: Doing Zero Out of the current spectrum for all values below 10 is done by:

```
SpecMath.Zero(Specbar.CurrentSpectrum,10);
```

8.1.10 Normalize Amplitude

This command muliplies the values of a spectrum by an overall constant so that the amplitude of the spectrum is normalized, that is in such a way that the maximal value of the spectrum is set to a normalization value that is specified in a dialog box.

JScript Syntax: Normalizing the current spectrum to 1 is done by:
`SpecMath.NormalizeAmplitude(Specbar.CurrentSpectrum,1);`

8.1.11 Normalize Energy

This command normalizes the area under the graph of the spectrum in the active spectrum sheet to the value that is entered in the dialog box. This is especially useful if you want to convolute as the convolution is not supposed to affect the order of magnitude of the spectral values. Considering this it is necessary to normalize the convolution core. In other words its area has to be one. Through this you can for example take the spectral line of a mercury lamp as a convolution core, normalize the surface area by using "normalize energy" to one and then convolute the line.

The algorithm works as follows: All values of the channels within the math range are summed up and one obtains the area (energy) E_{before} ("'discrete integration"'). Then the spectrum is multiplied by the ratio E_{set}/E_{before}, where E_{set} is the Energy specified in the dialog box.

JScript Syntax: Normalizing the area under the graph of the current spectrum to 1 is done by:

`SpecMath.NormalizeEnergy(Specbar.CurrentSpectrum,1);`

8.1.12 Bias Adjust

This command just subtracts the average of the values of the spectrum from the values within the math range.

Warning: *The average of the spectrum is not calculated in respect to the math range, but the overall spectrum.*

JScript Syntax: Adjusting the bias to the average of the values of the current spectrum is done by:

`SpecMath.BiasAdjust(Specbar.CurrentSpectrum);`

8.1.13 Ring spectrum

This command shall be used for spectra which were recorded by using sun light. In this case, the so called ring effect has to be corrected. The ring effect is due to the Frauenhofer lines in the sunlight.

JScript Syntax: The ring spectrum is calculated using

```
Scattering.CalcRingSpectrum(Specbar.CurrentSpectrum);
```

with the following default values: Temperature: 250K, JMax: 30, Mixing: 0.8, SZA: 90. One can of course specify these values:

```
CalcRingSpectrum(specOrig, 250, 30, 0.8, 90);
```

Warning: *The ring spectrum can of course only be calculated if the spectrum has wavelength information.*

8.1.14 Dark Current and Offset

Dark current and offset corrections are important to reduce the error that is due to CCD imperfections. Dark current effects arise for example because of the finite temperature of the chip (thermal excitations of channels occure), offset effects arise because of readout imperfections. Therefore, before and after a series of measurements, a dark current spectrum (one scan with high exposure time) and a offset spectrum (high number of scans and very short exposure time) should be recorded.

The Correct Dark Current command subtracts the dark current spectrum from the spectrum to which it is applied in the so called time-weighted mode; compare spectrum operations

The Correct Offset command subtracts the dark current spectrum from the spectrum to which it is applied in the so called scan-weighted mode; compare spectrum operations

8.1.15 Convolute

The Convolute command convolutes a cross section spectrum with the instrumental function that has to be specified in a dialog box.
A convolution (german: Faltung) is smearing out a given spectrum, using the so-called kernel, which usually is the instrumental slit function. For example, a theoretical calculation of a spectrum (or a spectrum recorded under ideal conditions, with a delta function as the slit function) is convoluted to compare it with the measured spectrum.
Convolution can be done both on wavelength or channel-basis.
The kernel is defined by the math range of a spectrum. The center of the kernel function and therewith the origin of the convolution kernel is the center of the math range A cubic spline is used to get a continuous function of the kernel.

JScript Syntax: Convolution is done by using:

```
SpecMath.Convolute(ISpectrum specSource, ISpectrum specKernel,
ISpectrum specTarget, ConvolutionKernelMode ckmKernelMode);
```

where ConvolutionKernelMode is either ConvolutionKernelMode.Normal or ConvolutionKernelMode.Normalize, where the second mode is used when the kernel shall be normalized before convolution.

8.2 Navigate an Open Spectrum

8.2.1 Move and Zoom

By default, a spectrum will be displayed in the entire range, e.g. 1024 channels (exception: spectrums in the Fit Result window, which are displayed in the fitting range).
You can zoom into the spectrum by drawing a box of a width corresponding to the range that shall be displayed. By clicking the right mouse button, you zoom out to the entire range again.

Hint: You can shift the range that is displayed by one channel by pressing the `left` or `right` key. You can shift it by 10 channels by pressing `page up` or `page down`.

8.2.2 Markers

There are four types of markers:

- The marker consists of It is useful to display the value of a certain channel (which is displayed when moved) or for acquiring coordinates (e.g. in the calibration assistant).
- The math markers (for determining a math range)
- The fit markers (for determinig a fit range)
- The optical density marker (for determining a range to calculate the optical density)

All markers are moved by dragging and dropping it in the *lower part of the spectrum*. They can also be moved channelwise by pressing `Strg-left` or `Strg-right`. If more than one marker is visible, this is applied to the marker that was moved last.