Analysis of spectral wavelength shifts, spectral anomalies, spectral resolution and calculation of weighted UV-doses by means of the software package SHICrivm

USERS GUIDE (concept July 2002): SHICrivm version 3.075; developed within the context of the project Scientific UV data management SUVDAMA (4th framework program) and the project European Database for Ultraviolet radiation Climatology and Evaluation (EDUCE); to be applied under the co-operative agreement of the 5th framework EC-project EDUCE.

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Abstract

The SHICrivm software package was developed over the past years aiming at improving the comparability of data sets obtained with different spectral instruments, and as a QA/QC-tool for checking or calibrating spectral wavelength shifts. The methods have been extensively tested for a wide variety of instruments in the context of several large scale intercomparison campaigns, and in routine monitoring. The SHICrivm software package combines several routines and includes the following functionality:

- a determination of wavelength dependent spectral wavelength scale errors/shifts of the measured solar UV-spectrum by comparing the spectral strucutre with a hiogh resolution extraterrestrial spectrum (shift determinations on 16 nm intervals from 290 nm up to 600 nm are possible; analysis up to 400 nm extensively tested)
- alignment of the measured solar spectrum, correction of the wavelength error/shift
- deconvolution of the measured spectrum (using the user-specified slit function or a triangular slit with user specified Full Width at Half Maximum FWHM)
- calculation of a spectrum corrected for wavelength shifts, and calculation of a standardised 1 nm FWHM spectrum (the latter two are based on the deconvolved spectrum)
- calculation of effective UV for a set of action spectra, and irradiances integrated over a set of wavelength intervals (using the deconvolved spectrum)
- check of the spectral structure, identifying possible (local) spectral anomalies (spikes in a spectrum)
- identification of the lowest irradiance levels where the readings become reliable, including the determination of the "starting" wavelength where readings become reliable
- full EDUCE-quality flagging: for wavelength shifts (spectral and integrated in two wavelength regions); flagging for spikes and spectral shape errors; flagging for lowest irradiance and starting wavelength of the spectrum; flagging for (cloud) variability during the scan
- identifaction of cloud-transmission and cloud varibility during the scan
- calculation of spectral atmospheric transmission

For users who want to follow the shortest route to applying the software package we refer to the section 2 : **A quick route to the installation and use of SHICrivm**. In that section four steps are described to install and use the package for one or multiple spectral data files. The whole procedure should take no more than 15 minutes. When the SHICcall windows shell is used the results of wavelength shift determinations, spectral distortions, transmissions can be shown in a plot on the screen using the view button.

Section 3 gives details on the application of SHIC and section 4 on the specification of input. The reading of those sections is probably not necessary for all users. The output is specified in section 5 and a summary of QA/QC results is given in section 5.4.

All routines are developed at RIVM, for which Harry Slaper is the primary contact.

1 Introduction and Short Background information

1.1 General

Spectral measurements of solar UV put high demands on the accuracy of the wavelength calibration, because deviations of the order of 0.03-0.05 nm easily cause errors of the order of one percent in the calculation of biologically effective UV. In view of the fact that the routine monitoring usually occurs with wavelength steps of 0.5 - 1 nm the accuracy of the wavelength calibration should typically be one tenth of the wavelength step. The Fraunhofer structures in the solar spectrum can be used for a highly accurate wavelenght alignment of spectra. The methodology developed at RIVM, and reported by Slaper et.al. 1995, was improved within the SUVDAMA and EDUCE projects, and now allows for routine evaluations of spectral dependent waveelength shifts and spectal shape errors. In addition the routines provide an indication of possilble irradiance scale errors.
The methods have been successfully applied in most large international intercomparison campaigns in the past years, among which CAMSSUM95, NOGIC96, NOGIC2000 and SUSPEN97, MAUVE/CUVRA1999, QASUME_2002 and two smaller campaigns. Thus, much experience was gathered for a wide variety of different instruments. The methods have now been adjusted so that they can be used for routine monitoring, and are included in the SHICrivm software package.

1.2 Background

Differences in the slit function, particularly in the FWHM, cause a reproducible spectral 'noise' when spectra from different instruments are compared. Deconvolution techniques can, at least partly account for these problems in comparing data from different instruments. The techniques used here have been described elsewhere: Slaper etal 1995, Slaper 1997, Slaper and Koskela 1997. Following the deconvolution a convolution is conducted to obtain a spectrum based on a virtual instrument with a FWHM of 1 nm (using a triangular slit function). In addition to this standard spectrum also the shift corrected spectrum with the slit function of the measuring instrument is provided.
The deconvoluted spectrum is used to calculate effective UV for various (user specified) action spectra and for certain wavelength intervals.
During the intercomparison campaigns it was noted that occasionally instrumental readings contain large spectral anomalies (spikes) due to erroneous readings. The software package includes a routine that checks and reports large discrepancies in the spectrasl structure of the measured spectrum.. Large spectral anomalies can cause erroneous shifts and deconvolution, however this is shown and reported in the spectral shift files by means of large error ratios. Data files where some readings are omitted can be directly re-analysed by the SHIC-software.

1.3 About this document

This document describes both the installation and use of the programs, as well as a specification of the major input parameters and the output produced. A quick route to the installation and application of the programs (section 2) is provided. Reading and applying chapter 2 should cover most standard use of the package. More detailed information on the possible application and input is given in sections 3 and 4 respectively. Section 5 summarises the major output of the program package; the QA/QC aspects are mainly dealt with in section 5.4. This guide does not provide an extensive description of the options available in the programs, and the full flexibility contained in the present version of the package.

The package contains a windows user shell SHICcall (version 5.20 or higher) which can be used for running one spectrum or multiple spectra in one run, and which can also be used to easily install the package for the evaluation data from new instruments, or to alter the main installation settings. In addition the user shell allows a direct view of the major results obtained: spectral wavelength shifts, spectral shape errors, diurnal variation in shifts for two wavelength regions and a diurnal spectral shape parameter to quickly identify spectra with potential problems.
The dos-user shell RUNshic.bat, which was included in the previous release (version 2.79) is not included in the present package. If required the old version could still be used from the 2.79 package, however using the new windows shell is recommended.

1.4 Conventions

Throughout the document LLL will be used as the instrument identification (any three letter/number code could be used). All input/output specifically related to the instrument will be identified with the LLL-code in the filenames. Files with the extension dfa, are used by the programs to set parameter

'defaults'. Data files should be named: DDDhhmm.LLL, where DDD-day number in the year, hh –hour (normally UTC, but other time zones can be used), mm -minutes). The LLL.sli file gives the slit function data.

Default paths:

c:\SHICrivm\UVDATA\
the main datapath, here or in a subdirecotry the measured spectral data files should be present; default the spectra are in the LLL subdirectory under this path, and the full data path refers to: c:\SHICrivm\UVDATA\LLL\
datafiles according to the name convention: DDDhhmm.LLL
nb longer filenames than 7.3 are possible: DDDhhmmXXXXX.LLL, however not all further analysis will be consistent with the further identification XXXXX.

c:\SHICrivm\UVANALYS\
the Main Analysis datapath: the path should exist prior to running SHICcall! The slitfunction file LLL.sli should be available in this directory. Following installation here also the instrument specific defaults (usually LLL.dfa) and the main program defaults will be located.

Program and default input paths:
c:\SHICrivm\SHICcall\
start SHICcall5_25.exe or later from this directory;

c:\SHICrivm\UVANALYS\etoz\
Extraterrestrial solar spectrum, ozone cross section and action spectra.

In default settings all measured UV-data from the instrument should be in the UVDATA\LLL directory. The user can change this setting from the user shell. This path is referred to as the Full data path. The main analysis path refers to the UVANALYS directory in default settings. This main analysis path contains some files that control the settings of the analysis, the instrumental characteristics and the slit function (named LLL.sli). All analysed data are provided in the UVANALYS\LLL subdirectory (ie in the subdirectory LLL under unvanalys). DDDhhmmi.LLL files (for example 1621030i.NLR) provides the shift corrected spectral irradiances for a standardised slit function (FWHM 1.0 nm)) and the wavelength corrected spectral irradiance for the instrument specific slit function. Detailed shifts are reported in the LLL\SHIFT directory; effective UV for several action spectra is given in the LLL\efuv; and some QC summary results are provided in the QAQC subdirectory (flagging, wavelength shift summary, structural errors report). Spectral shape errors and comparison with clear sky transmission estimates are provided in the STRUC subdirectory under the QAQC directory. An overview of spectra in the various flagging categories can be found in the QAQC directory, in the DDDQflag.LLL files. Detailed spectral information on the atmospheric transmission is provided in the TRANS subdirectory.

1.5 Requirements

The package should work on DOS and Windows based Pentium-PC's with Windows 95, 98, NT, XP, with at least 64 MB RAM.

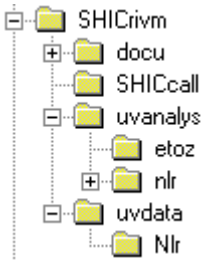
2 A quick route to the installation and use of SHICrivm

2.1 Quick installation

2.1.1 for new users

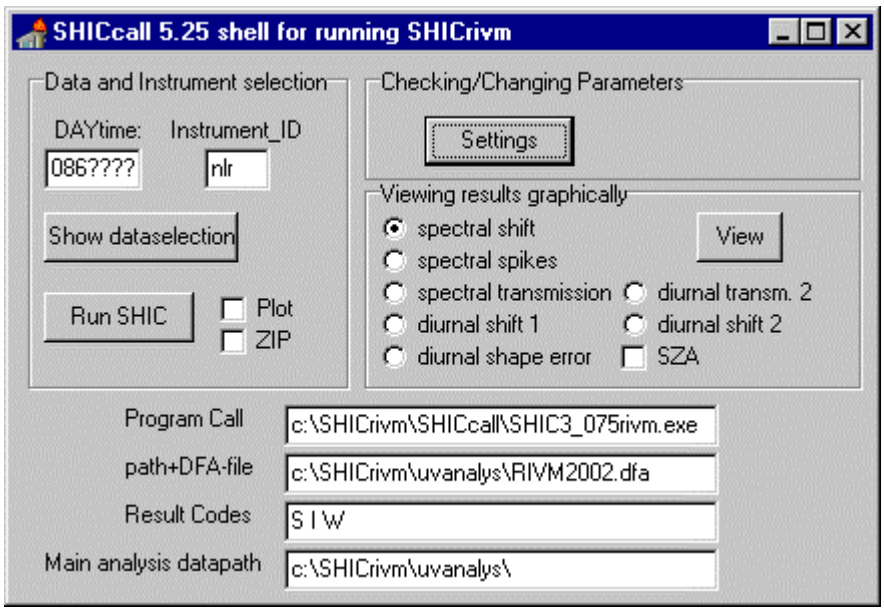
We have now provided a standard installation for the EDUCE project which should make the programs easy to use. The package is contained in a zip-file and running requires the following 4 steps:

step 1 unzipping the files and directory structure: unzip the file and directory structure; following installation teh following main directory structure should exist:

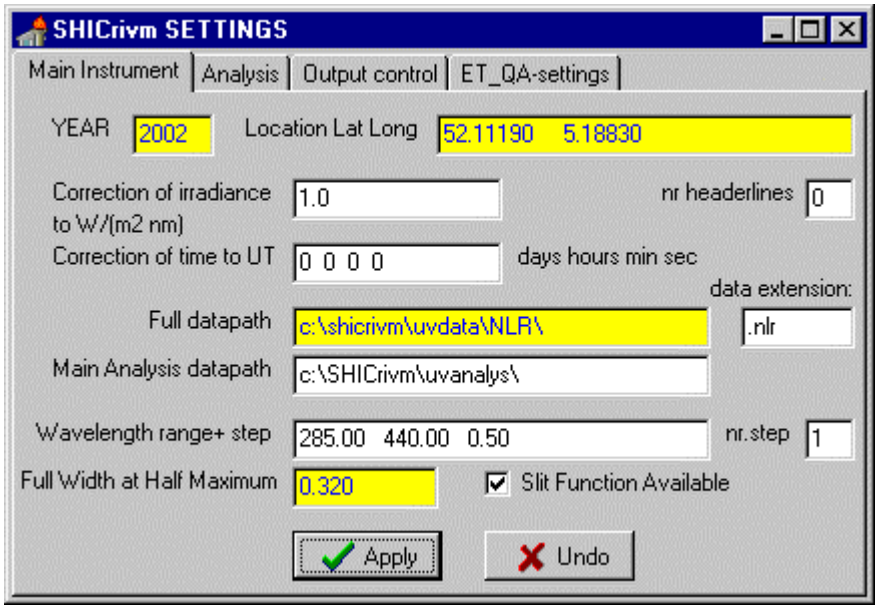


step 2 copy the measured spectra and slit function to the appropriate directories set in shiccall, defaults: data in c:\SHICrivm\uvdata\LLL\; slit function in main analysis path: c:\SHICrivm\uvanalys\. (NLR-example is pre-installed)

step 3 Run SHICcall, set the parameters for the specific instrument and the measurements to be analysed (DAYtime field and instrument-ID (LLL-code)) and the paths and the main analysis datapath (path should exist!) and DFA-file name (file can be created by SHICcall)
Main SHICcall window: here all spectral data-files from day 086 for instrument nlr will be analysed

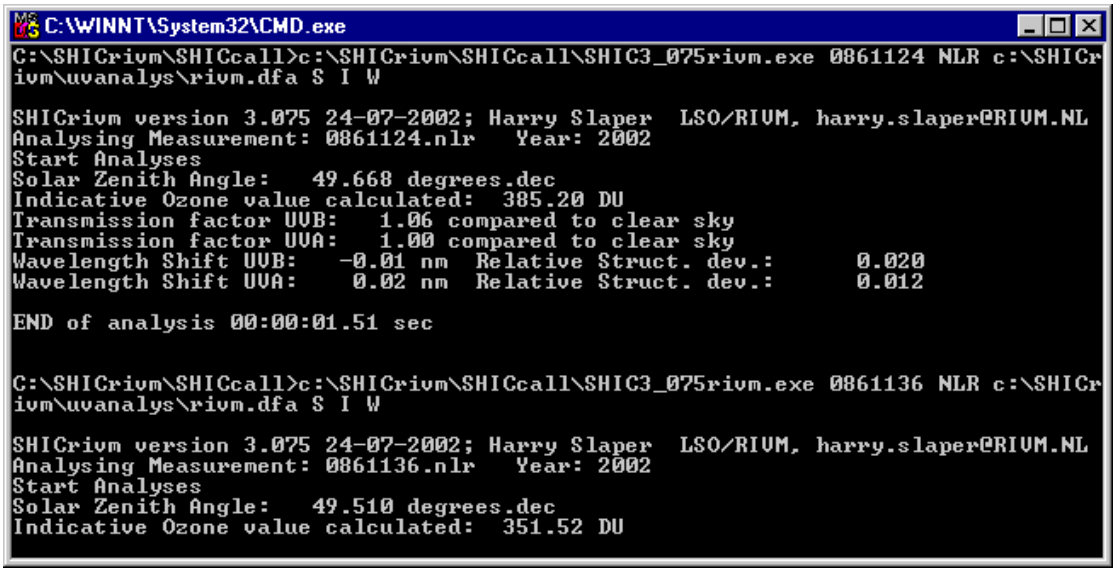


Use the settings button to adjust parameters like the year of measurement, the location (Latitude, Longitude in degrees decimal) settings on wavelength range of measurements (confirm changes by pushing apply buttons). Example of main settings page:



step 4 push the RUN button in the SHICcall main page.

Example of the SHIC3_075rivm.exe run-window. Run starts with version line: SHICrivm version…. Then gives the analysed filename (DDDhhmm.LLL, inthis case 0861124.nlr), information on the estimated transfer in the UVA and UVB and the wavelength shifts in these regions. End of analysis indicates a successfull end of the run (this run was on a 300 MHz Windows NT-pc).



2.1.2 Users with a pre-installed version 2.79 or 3.03x

Previous users of the version 2.79 can take a quick route to install the new version. Just copy the files indicated in the SHICcall directory and the etoz directory to the appropriate directories. Start SHICcall5_20 and adjust the settings (paths and filenames) according to the al ready available installed version.
Program and default input paths:
c:\SHICrivm\SHICcall\

following installation this directory should contain at least:

Efuv.dfa	1KB	DFA File	19-6-02 11:23
Pkzip.exe	42KB	Application	1-2-93 2:04
shic_bat.bat	6KB	MS-DOS Batch File	24-7-02 14:14
Shic_e.dfa	3KB	DFA File	20-6-02 11:55
SHIC3_075rivm.exe	190KB	Application	24-7-02 10:12
SHICcall.dfa	1KB	DFA File	24-7-02 13:49
SHICcall5_25.exe	568KB	Application	20-7-02 15:12
shicrivm.log	114KB	Text Document	24-7-02 14:17
shift.log	108KB	Text Document	24-7-02 14:17
View2.exe	492KB	Application	16-6-02 13:03
viewer.dfa	1KB	DFA File	24-7-02 15:48

Extraterrestrial solar spectrum, ozone cross section and action spectra; default path:
c:\SHICrivm\UVANALYS\etoz\

default content at least:

kp320a3L.1nm	231KB	1NM File	30-4-02 17:24
kp320a3L.et	1,032KB	ET File	16-4-02 8:26
Mckinlay.dat	5KB	DAT File	6-8-94 9:34
O3cross.wgt	31KB	WGT File	16-10-94 22:16
Peakkub.dat	5KB	DAT File	6-8-94 9:39
Rb_new.dat	1KB	DAT File	6-8-94 9:42
Rb_old.dat	5KB	DAT File	6-8-94 9:38
scup_h.dat	4KB	DAT File	23-4-97 17:28
Scup_m.dat	5KB	DAT File	6-8-94 9:28
Stesla.dat	5KB	DAT File	6-8-94 9:32

2.2 Installation details

Step 1
Copy SHICzip.zip to a directory which will be used as the main directory (for instance: c:\SHICrivm\) and unpack the package and the subdirectories using pkunzip/winzip or a similar unzip-program.
Recommended main path (other paths are possible):
c:\SHICrivm\
It is recommended to keep the path and filenames in the DOS-convention: 8.3 (datafiles 7.3). The program could run with longer filenames, however the user should be aware of potential ambiguity in some of the output, because daily files are indetified only by the DDD (day-nr) code.

The programs, data files and the following standard directory structure will be created automatically:

c:\SHICrivm\UVDATA\	{Measured data should be here, in simple two column format}
c:\SHICrivm\UVDATA\NLR	{Here you find three example measurements for the NLR-instrument}
c:\SHICrivm\UVANALYS\	{Contains files with parameter settings; slit function}
c:\SHICrivm\UVANALYS\ETOZ\	{Contains ET-spectrum, O3 cross sections and action spectra}
c:\SHICrivm\SHICcall\	{Contains SHICcall and shicrivm main program}

A check, or example calculation could be performed using the pre-installed NLR data. In the latter case go directly to step 3.

Default paths:

c:\SHICrivm\UVDATA\
the main datapath, here or in a subdirecotry the measured spectral data files should be present; default the spectra are in the LLL subdirecotry under this path, and the full data path refers to:
c:\SHICrivm\UVDATA\LLL\
datafiles according to the name convention: DDDhhmm.LLL (example: 1621030.NLR)
nb longer filenames than 7.3 are possible: DDDhhmmXXXXX.LLL, however not all further analysis will be consistent with the further identification XXXXX. DDDhhmm.LLLyyyyy will also be correctly analysed by SHIC, and all extensions will also appear in the analysed output-files, hoiwever the zipping-procedure in SHICcall will not work properly if the 7.3 data-format is not used.

c:\SHICrivm\UVANALYS\
the Main Analysis datapath: the path should exist prior to running SHICcall! In this directory the LLL.sli (slit function file should be available).

Program and default input paths:
c:\SHICrivm\SHICcall\
following installation this directory should contain at least:

Efuv.dfa	1KB	DFA File	19-6-02 11:23
Pkzip.exe	42KB	Application	1-2-93 2:04
shic_bat.bat	6KB	MS-DOS Batch File	24-7-02 14:14
Shic_e.dfa	3KB	DFA File	20-6-02 11:55
SHIC3_075rivm.exe	190KB	Application	24-7-02 10:12
SHICcall.dfa	1KB	DFA File	24-7-02 13:49
SHICcall5_25.exe	568KB	Application	20-7-02 15:12
shicrivm.log	114KB	Text Document	24-7-02 14:17
shift.log	108KB	Text Document	24-7-02 14:17
View2.exe	492KB	Application	16-6-02 13:03
viewer.dfa	1KB	DFA File	24-7-02 15:48

Extraterrestrial solar spectrum, ozone cross section and action spectra; default path:
c:\SHICrivm\UVANALYS\etoz\

The default content should be at least:

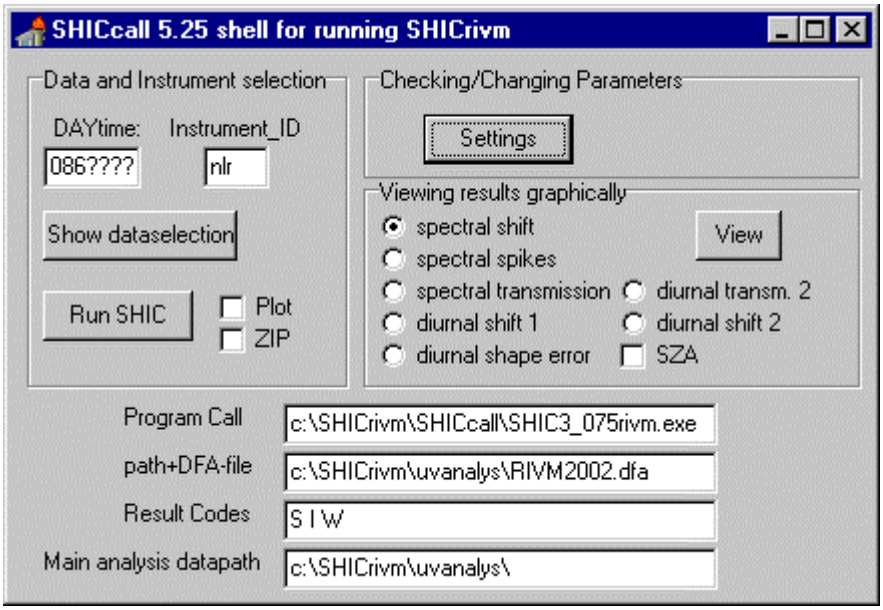
kp320a3L.1nm	231KB	1NM File	30-4-02 17:24
kp320a3L.et	1,032KB	ET File	16-4-02 8:26
Mckinlay.dat	5KB	DAT File	6-8-94 9:34
O3cross.wgt	31KB	WGT File	16-10-94 22:16
Peakkub.dat	5KB	DAT File	6-8-94 9:39
Rb_new.dat	1KB	DAT File	6-8-94 9:42
Rb_old.dat	5KB	DAT File	6-8-94 9:38
scup_h.dat	4KB	DAT File	23-4-97 17:28
Scup_m.dat	5KB	DAT File	6-8-94 9:28
Stesla.dat	5KB	DAT File	6-8-94 9:32

step 2 copy the measured spectra and slit function
Copy the slit function to the Main analysis directory (usually c:\SHICrivm\UVANALYS\).
Copy the spectral measurements to the Full datapath directory, usually: c:\SHICrivm\uvdata\LLL\

In default settings all measured UV-data from the instrument should be in the UVDATA\LLL directory. The user can change this setting from the user shell. This path is referred to as the Full data path. The main analysis path refers to the UVANALYS directory in default settings. This main analysis path contains some files that control the settings of the analysis, the instrumental characteristics and the slit function (named LLL.sli).

step 3 Run SHICcall, set the parameters using the settings button

Goto the SHICcall subdirectory and start the SHICcall program. The opening screen should look similar to:



DAYtime should provide the DDDhhmm name-code for the specta to be analysed. Using the usual DOS/windows convention with question marks and * makes it possible to select multiple files (if filenames are longer than the default 7 digits of the DDDhhmm code use * as last digit).

Instrument id: three lettercode LLL (in example above nlr is chosen).

Make sure the **Program Call** points to the correct path and executable name: SHIC3_065rivm.exe (this can be any path wanted).

path+DFA-file should point to the main analysis file and you should give a logical name for the defaults settings, in the example RIVM.dfa is chosen to represent the settings for the RIVM location and other parameters. It is not necessary that this file exists before running SHICcall. However, the path should exist prior to running or installing! Advice: give a name longer than 4 symbols and use .dfa to isdentify the file as default settings file.

Result codes usually should not be changed: S refers to the extension of the output of the detailed spectral shifts (DDDhhmmS.LLL) produced after running SHIC (in the directory: LLL\shift\). Result code I refers to the analysed irradiance (DDDhhmmI.nlr, in directory LLL\). Result code W refers to the spectral shift, which is applied in the analysis for each wavelength in the measured spectrum (in the directory LLL\shift\). The program allows additional parameter settings in the result codes (in one additional string without spaces):

- no_sh_cor implies that the calculated shifts will not be used in the deconvolution analysis
- spike_cor implies that SHIC will check and correct for spectral spikes (in deafult settings spikes exceeding a factor of 2 will be adjusted)
- spike_cor_no_sh_cor is also possible if a combination of both options is wanted

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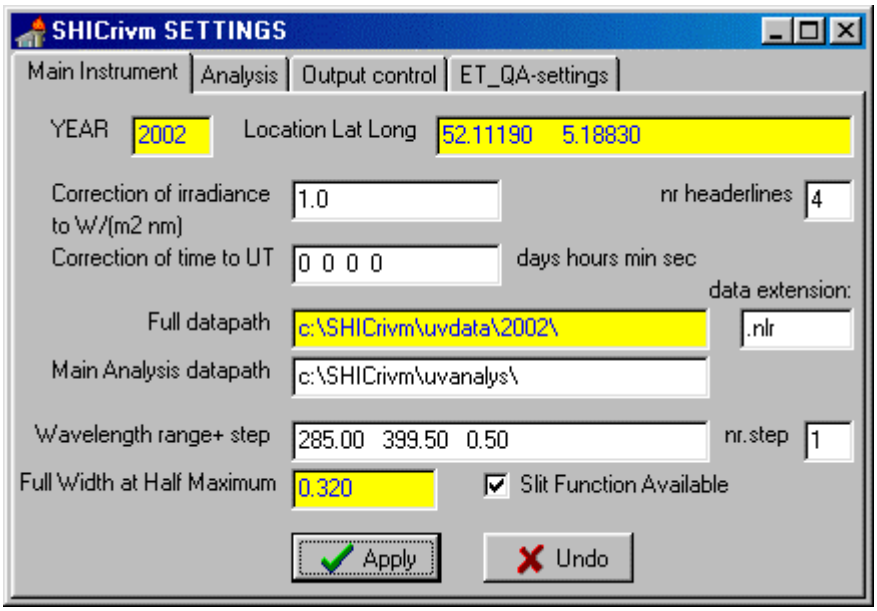
Main analysis datapath: it is important that this analysis datapath exists prior to running. It is good practice to use the same path for the path+ dfa-file.

Push the SETTINGS button:



Adjust the **YEAR**, and **location** settings to accommodate the settings for the data to be analysed. Check and adjust the **Full datapath** (path for the spectra data), and the **Full Width at Half Maximum** for your instrument. Is the slit function available? (clicked implies the **Slit function is available**).
The SHIC program expects the spectral irradiance in the unit Wm^{-2} /nm. If you use an other unit provide the **correction of irradiance** factor required to obtain the standard SHIC-unit.
The SHIC program expects the time in UT. If you use local time elsewhere, you can provide the **Correction of time** to UT, which should consist of 4 numbers: the number of days, hours, minutes and seconds (use integer numbers separated by spaces). The time given is added to the DDDhhmm time in the filename convention (this is used to calculate the solar zenith angle). Correction of time can be used to adopt to different time-zones, and if required to calculate the time during the scan rather than the time at the start of the scan.

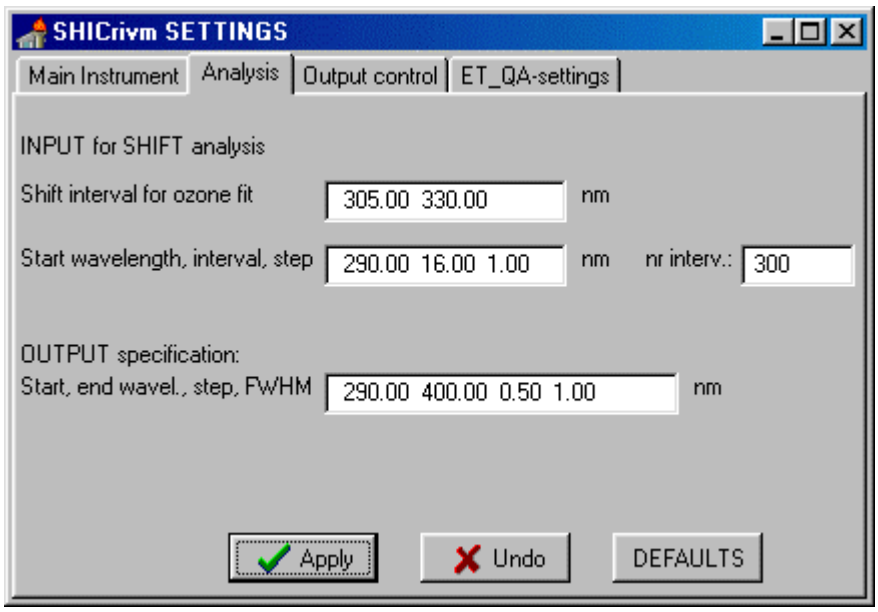
All analysed data are provided in subdirectories of the **Main analysis datapath**, default in the UVANALYS\LLL subdirectory (ie in the subdirectory LLL under unvanalys) It is good practive to change this path only on the Main page.

The datafiles should have at least two columns of data and the first two columns should be: the wavelength in nm and the spectral irradiance (Wm^{-2} /nm). The two columns can be preceded by a number of **headerlines**, and the number of headerlines could be indicated. The latter is required if the headerlines contain numbers in the first two positions. The headerlines, if a number larger than 0 is given, will appear in the headerlines of the output files.
The **data-extension** refers to the extension of the data-files (include the point!) and usually this refers to the LLL-code for the instrument.

The **nr_step** parameter refers to the (integer) number of wavelength steps between the irradiance datapoints that are intercompared to check the structure and determine the wavelength shift. A rule of thumb is that nr.step is the integer number larger than 0 and closest to: FWHM/(2 x wavelength_step).

After changing settings **APPLY** should be clicked to apply the altered settings!

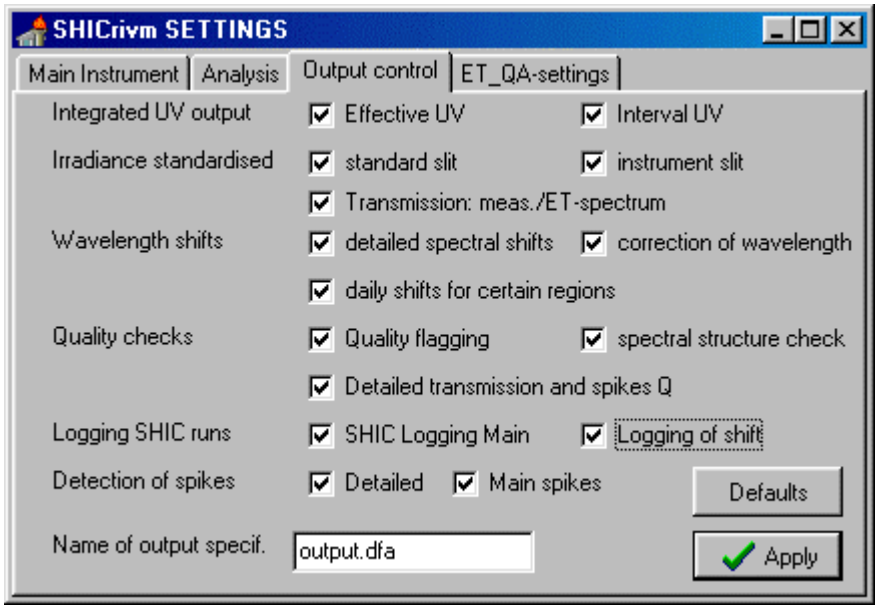
Analysis settings
If specific analysis settings are required the second tab of the Settings page could be clicked. If standard output is requiered this is not necessary. The analysis page looks like:



The **Shift interval for ozone fit** edit box gives the range of the wavelength interval that is used to get an indication of the ozone absorption in the atmosphere. It should be noted that the ozone value calculated is no more than an indicative value, and has no pretention to be an accurate ozone estimate.
The **start wavelength, interval and step** settings give the starting wavelength of the first interval on which the shift is determined, followed by the wavelength interval applied, and the wavelength step (all in nm) to the next interval. The **nr.interv**. edit box indicates the maximum number of intervals that will be analysed.

The **Output specification** provides the wavelength interval, the wavelength step and the Full Width at Half Maximum of the analysed spectral irradiance output (which is given in the DDDhhmmI.LLL files in the uvanalys\LLL subdirectory).

OUTPUT CONTROL tab in the SETTINGS page
Detailed settings of the output files can be made on the output control tab page.

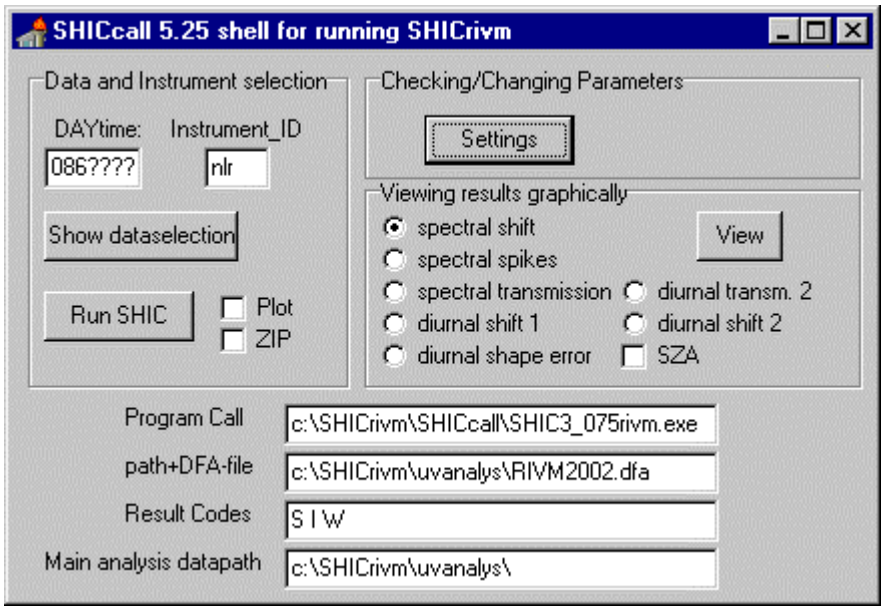


DDDhhmmi.LLL files (for example 1621030i.NLR) provides the shift corrected spectral irradiances for a standardised slit function (FWHM 1.0 nm)) and the wavelength corrected spectral irradiance for the instrument specific slit function. Detailed shifts are reported in the LLL\SHIFT directory; effective UV for several action spectra is given in the LLL\efuv; and some QC summary results are provided in the QAQC subdirectory (flagging, wavelength shift summary, structural errors report). Spectral shape errors and comparison with clear sky transmission estimates are provided in the STRUC subdirectory under the QAQC directory. An overview of spectra in the various flagging categories can be found in the

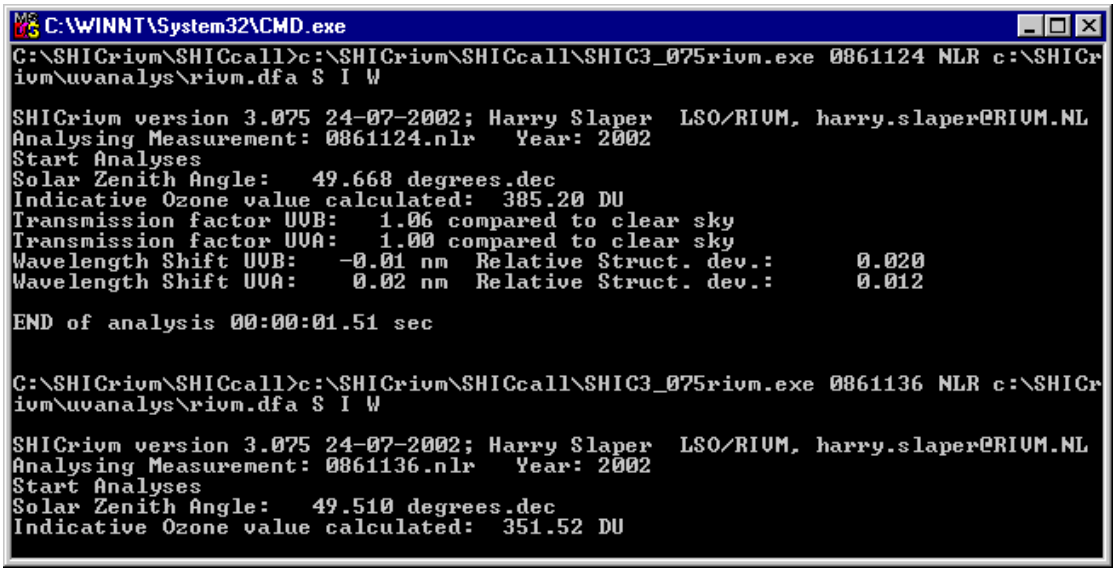
Detailed spectral information on the atmospheric transmission is provided in the TRANS subdirectory.

Step 4 RUN SHIC from the SHICcall main page

If the Settings have been adopted: close the Settings-pages. The main SHICcall page will show:



Push the Show dataselection button to see which datafiles are selected for the analysis. If no data is found change the settings. Push the run button to start an analysis of the selected datafiles. If a large number of spectra (>100) is selected it is adviced not to mark the plot button, because it will take a long time for the plot to be made. Results of the analysis can also be viewed afterwards by uysing the view buttons and selecting the type of plot wanted. Running the program will show for example:



2.4 Installing a new instrument

The SHICrivm program can now be installed from the user shell by changing the instrument ID, and the settingds. The following information on the instrument and location is required:

- year of the measurements to be evaluated
- Longitude and Latitude of measurements (degrees.decimal)
- Three letter code LLL (3L-code, any three letters/numbers, avoid GLE, DFA) for the instrument to be analysed. Results will have this LLL-code as an extension, and all results will be in a subdirectory under UVANALYS, which is identified by the LLL-code.
- Wavelength range measured: start and end wavelength (in nm) and wavelength step NB: Variable wavelength ranges and variable steps are properly handled, but the range should provide the maximum range (data outside the range are ignored in the analysis!)
- Full Width at Half Maximum (FWHM) of the slit function
- If possible the slit function should be available (in simple two column format with a zero at the nominal wavelength). If a spectral line or a laser line is used to determine the slit function the measurement should be mirrored in the nominal wavelength in order to obtain the slit function. The slit function file should have the nominal wavelength indicated with 0 (zero).

Start the SHICcall5_25 (or higher) user-shell. Fill the edit fields in the settings pages with the requested details, and push the apply button for changes to take effect.

2.5 Single spectrum evaluation (Use the SHICrivm program)

Data files should be in the UVDATA subdirectory, and according to the SHIC (SUSPEN) name and format convention.
Go to the Subdirectory SHICrivm\UVANALYS and start SHICrivm
An example of the standard program call:
SHICrivm 1621030 NLR c:\SHICrivm\UVANALYS\SHICrivm.dfa
or
SHICrivm 1621030 NLR c:\SHICrivm\UVANALYS\SHIC_e.dfa

where:
measurement at day 162 10.30 UT, for instrument NLR (Netherlands RIVM);
a short list of parameter values are in: c:\SHICrivm\UVANALYS\SHICrivm.dfa, an extended list of parameter settings is in SHIC_e.dfa.

The results of the analysis are given in UVANALYS\NLR and subdirectories:
- corrected and homogenised spectra irradiances are in UVANALYS\NLR\1621030i.NLR
- results of the shift analysis are in UVANALYS\NLR\shift
- results of the QA/QC summary on shifts and spectral irregularities are in: UVANALYS\NLR\STRUC

See section 4 for the details on the output, and for the use of additional software for data summaries and/or statistics.

A formal description of the SHICrivm program call:
SHICrivm [DDDhhmm] [LLL] <main path+default filename> <id_shift> <id_specout> <id_shif_appl>

[...]	- required input;
<...>	- optional (otherwise defaults in shicRIVM.dfa are applied); optional parameters are not required;
DDDhhmm	- DDD day number in year;hhmm hour minutes example: 0231225 (day 23, 25 minutes past 12;
LLL	- three letter code (3L-code) for instrument_identification; for example NLR
path+ default	- file with overall defaults, for example RIVM.dfa; see note below
id_shift	- identification (1 lettercode) for results of shift analysis; normal s
id_specout	- identification (1 lettercode) for analysed simulated spectra; normal i
id_shif_appl	- identification (1 lettercode) for shifts applied in analysis; normal w the latter provides interpolated shift values for each wavelength measured, if not specified results are in shiftlog.log;

Default value for id_shift is s, for id_specout is i, for id_shif_appl is w.
The file with default parameter should in not be LLL.dfa

3 Input specification for SHICrivm

3.1 Format for spectral data-file

SPECTRAL INPUT DATA

LOCATION:
in the subdirectory UVDATA\LLL (other paths are possible but should be specified in LLL.DFA file)

FILENAME (SUSPEN NAME CONVENTION):
DDDhhmm.LLL
where DDD is an identification of the day in the year, hh stands for hour in the day (UT), mm for minutes. An example of the filename: 0851224, stands for a spectrum measured on day 85 at 24 minutes past 12 hours (UT). LLL - stands for a three letter code to identify the instrument

FILE CONTENTS
- The data file can have a user-defined number of header lines. The standard installation can cope with any number of header lines, as long as the header lines do not start with two numbers. If one or more header lines do start with two numbers the number of header lines should be specified in the instrument specific default-file LLL.DFA, where LLL represents the instrument specific three letter code. This is done by specifying the nr of headerlines in the Settings page of SHICcall.
- Data lines contain at least two columns. The first two are used and should contain wavelength (in nm) and spectral irradiance (in any user defined units). Use spaces as separators, and Carriage Return at the end of the line (standard in most dos/windows-editors; from UNIX the use of UX2DOS might be required).

EXAMPLE CONTENTS
Header line 1 no problem if it does not start with two numbers
Header line 2 same
etceteras .....
285 0.00000E-0000
285.5 0.000001
286 0.00002e-1
.....
410 2.3e00

3.2 Instrument specific defaults

INSTRUMENT SPECIFIC DEFAULTS: LLL.DFA

This file is automatically created during standard installation, and can be adjusted manually (asc-II editor) or by a new installation.

LOCATION:
Subdirectory UVANALYS
FILENAME:
LLL.DFA, where LLL corresponds to the user defined instrument three letter code

FILE CONTENTS:
9 or 10 lines with parameter settings;
line 1: standard name for default file used in program (do not change)
line 2: number of header lines (0 in default, can be any integer number)
no_id_met indicates that the full path for the measurement is given in line 4, if omitted the program will expect the measurements in the subdirectory LLL under the path given in line 4
line 3: extension of the spectral data files (usually .LLL)
line 4: path where measurements are located (when no_id_met is omitted in line 2 this path will be extended with LLL)

line 5: wavelength range: start end and wavelength step (NB program only uses the wavelength range as a maximum range for the data, and the wavelength step (ws) as an indication. Variable ranges and variable steps (even within a data file are handled properly)
line 6: number (n) of wavelength steps (ws) between central and surrounding wavelengths used in shift algorithm; s = (n)x(ws) and should be approximately equal to the FWHM of the instrument
line 7: identification for slit function file availability: 0 - no file (use triangular slit); 1 - expects slit function file in subdirectory UVANALYS; name of slit function file should be: LLL.SLI
line 8: Full Width at Half Maximum (FWHM) of the slit function
line 9: 1 DO NOT CHANGE (larger number will lead to omission of data points from the analysis)
<line 10> A tenth line could be added to identify a unit-correction factor, which identifies a single factor with which all spectral irradiances are multiplied. The program expects the irradiance unit W/(m^2 nm) (if an other unit is used in the data-file use the unit correction factor to adjust to the standard SHIC unit).

EXAMPLE CONTENTS
ozonshi.dfa
0 no_id_met
.nlr
c:\SHICrivm\uvdata\NLR\
2.85000000000000E+0002 4.40000000000000E+0002 5.00000000000000E-0001
1
1
3.20000000000000E-0001
1
1.0

3.3 General default files for SHICrivm

Further parameter settings for the program are found in a second default file, which can have any name the user wants (with a few exceptions!). Do not use: LLL.dfa, efuv.dfa, output.dfa, LLL.sli or (when using SHICcall) do not use shicrivm.dfa. The latter dfa-file is shorter than the full general dfa-file and is created when the install option from the old SHIC-version is used. SHICcall will not properly work if SHICrivm.dfa is used. Users of the previous 2.79 version should rename their shic_e.dfa file and use that as general dfa-file (or make a new installation using the SHICcall5_20 shell.

When run the SHICrivm program will create SHIC_e.dfa which is an extended version of the general defaults and includes further internal and recommended defaults used in the program run. In addition a specification of the effective UV calculations is given in efuv.dfa (specified below).

GENERAL DEFAULTS: input data files

In addition to parameter settings the program requires input data, which are located in the subdirectory UVANALYS\ETOZ:

- a high resolution extra terrestrial spectrum KP320A3L.et is used as default (see RIVM contribution to the SUVDAMA final report)
- ozone cross sections (O3cross.wgt; derived from Bass&Paur, 1984)
- action spectra used in the calculation of effective UV: McKinlay.dat equals the CIE/IEC erythema action spectum from McKinlay and Diffey; SCUP_h.dat represents a skin cancer action spectrum for humans, derived from hairless mice action action spectrum accounting for different skin optics in human skin (de Gruijl and cvan der Leun 1994); SCUP_m.dat Skin cancer Utrecht Phildelphia action spectrum for hairless mice (de Gruijl etal 1993); STESLA.dat– older version of skin cancer action spectrum from Sterenborg and Slaper (Slaper 1987); PeakKUb.dat DNA damage action spectrum from Peak and Kubitshek; RB_new.dat sensitivity spectrum of newer type RB-meters; RB_old.dat sensitivity spectrum for older type RB-meters. Other action spectra could be used following proper specification in efuv.dfa (see below).

EFFECTIVE UV DEFAULTS FOR SHICRIVM: EFUV.dfa

This file provides the specification of the action spectra used in the effective UV calculations, and the intervals used for the calculation of the summed irradiance.

LOCATION: Subdirectory UVANALYS
FILENAME: EFUV.DFA, do not change this filename

FILE CONTENTS:
line 1: Number of effective UV output files: NR
Lines 2 and 3 are repeated NR-times:
line 2: 5 letter code to identify output of effective UV calculations
line 3: Maximum wavelength for effective UV calculation (nm)

line 2Nr+2: Number of action spectra evaluated: Na
line 2Nr+3 is repeated Na-times
line 2Nr+3: Filename of action spectrum data (action spectum file should be in c:\SHICrivm\UVANALYS\ETOZ)

line 2Nr+Na+3: 5 letter code to identify output of wavelength integrated spectral irradiance
line 2Nr+Na+4: Number of wavelength intervals for which integration is calculated: Nw
line 2Nr+Na+5 is repeated Nw times
line 2Nr+Na+5: start and end wavelength (nm) for calculated integrated spectral UV-irradiance

line 2Nr+Na+Nw+5: identifier for missing data, used in the daily files of results

The user can change the names and number of the action spectra and or the wavelength intervals required.

EXAMPLE CONTENTS
```
5
ef325
325
ef350
350
ef365
365
ef380
380
ef400
400
7
McKinlay.dat
Scup_h.dat
Scup_m.dat
Stesla.dat
PeakKub.dat
RB_new.dat
RB_old.dat
_step
10
300 310
310 320
320 330
330 340
340 350
350 360
360 370
370 380
380 390
390 400
 *
```

4 Output specification of SHICrivm and summary statistics

Output of the program for the user is available in a number of asc-ii files and can be found in analysed data files, and log-files. A brief description of the main output-files. The output files are found in subdirectories under the main analysis directory. In the default installation the main analysis directory is SHICrivm\UVANALYS\. In that main analysis directory a subdirectory is created which is identical to the instrument identification (3-lettercode LLL) in the program call given in the previous sections.
In the example the subdirectry will be NLR\.
All output is found in three four directories under UVANALYS\LLL :

- LLL\ i-spectra: corrected and homogenised spectral output DDDhhmmi.LLL
- LLL\SHIFT\; s-spectra: detailed spectral wavelength errors
- LLL\QAQC\ QA/QC results, flagging of analysed spectra in DDDQflag.LLL, summary on shifts; spikes, transmission etc in quality control data-files: DDDQC.LLL
- NLR\QAQC\struc\ q-files: spectral transmission compared to clear sky estimate and an identification of local spikes
- NLR\QAQC\flagstat\ summary files showing all spectra in overall flagging categories, taking the worst flag for each of five flags (shift1, shift 2, starting irradiance flag, transmission 2 flag, and spike and local shape flag), leading to: BLACK.LLL, GREY.LLL, RED.LLL, YELLOW.LLL, GREEN.LLL, and separately also files with spikes are identified in SPIKES.LLL (black or corrected on spike and local shape flag)
- NLR\EFUV\. Effective UV and wavelength range integrated UV; files usually
- NLR\TRANS\ t-files: Transmission of the atmosphere: measured irradiance/ET-irradiance (accounting for effects of the earth-sun-distance): DDDhhmmT.LLL

4.1 Flagging of quality parameters

The QAQC subdirectory contains information on the quality flagging of the spectra. The files DDDQflag.LLL contain the summary of all flagging. The general approach is as follows:

- spectra that meet the highest quality standard on a flagging criterium are flagged GREEN,
- spectra meeting somewhat lower quality/deviation setting: YELLOW,
- spectra flagged RED might have some severe deviatons,
- spectra flagged BLACK are unacceptable for most use,
- spectra marked GREY means that the algorithm was not fully conclusive, results were either not significant, or BLACK but they occurred at low irradiance levels (310 nm levels below 1e-4 W/(m^2 nm)).

shift1_flagging refers to the average wavelength error (shift) in the wavelength below 325 nm; if the calculated error is less than 0.10 nm the flag is green, from 0.10 to 0.20 the flag is yellow, from 0.2 to 0.4 nm the flag is red and >0.40 nm the flag is black; if the algorithm is not providing a significant estimate the flag is GREY; the flag is also GREY if the analysis leads to a BLACK result and the irradiance level is below 1e-4 W/(m^2 nm).

shift2_flagging refers to the average wavelength error (shift) in the wavelength range from 325 to 400 nm; if the calculated error is less than 0.10 nm the flag is green, from 0.10 to 0.20 the flag is yellow, from 0.2 to 0.4 nm the flag is red and >0.40 nm the flag is black; if the algorithm is not providing a significant estimate the flag is GREY; the flag is also GREY if the analysis leads to a BLACK result and the irradiance level is below if the algorithm is not providing a significant estimate the flag is GREY; the flag is also GREY if the analysis leads to a BLACK result and the irradiance level is below 1e-4 W/(m^2 nm).

Start_irradiance_flag: refers to the irradiance level at which the readings start to become significant (noise in the spectrum below 25% of the signal). The level is defined by the highest irradiance at or below the first wavelength of a series of five ratios of successive irradiance readings are within 25% of the expected ratios. If the so-defined spectral irradiance level is below 5e-4 W/(m^2 nm) the flag is GREEN, above this level but below 15e-4 W/(m^2 nm) the flag is YELLOW, above this level but below 50e-4 W/(m^2 nm) the flag is RED, above 50e-4 W/(m^2 nm) the flag is BLACK. The GREEN flag as defined here corresponds with the WMO guideline where the noise level should be such that 5e-5 W/(m^2 nm) corresponds to signal to noise ratio of 1.

Spike and local shape; this flag checks local deviation from the expected spectral structure, it is derived from a combination of two flags: the spike_flag_median_based, and teh local shape_flag. Spikes are identified and if a spectral irradiance reading deviates more than a factor of two from the expected irradiance compared with the five neighbouring readings the reading is called a spike and the spike flag turns black. If above the starting irradiance level (see above) more than 50% deviations occur among the ratio of two neighbouring spectral irradiances (compared to the modelled ratio), the flag will become RED, and th flag will become YELLOW if similarly the ratio deviates more than 25%.

Transmission 2 refers to the average transmission from 325 to 400 nm, which is around 1 for cloudless sky. This flag could be influenced by natural conditions (high mountains, snow albedo, low aerosol loads, clouds). If the transmission is between 0.1 and 1.25 the flag is GREEN, above 1.25 below 1.5 the flag is YELLOW, above 1.5 below 2 the flag is RED, and above 2 the flag is BLACK. With low transmissions the YELLOW flag is used with transmissions between 0.05-0.10, the RED flag between 0.01 and 0.05, and the BLACK flag below 0.01 transmission. If the flags are BLACK it is highly likely that an error occurs in the wavelength scale, yellow and red flags could occur occasionally.

The scan-variability_2 indicates variations in the transmission for wavelength range 2 during the scan: this flag primarily focuses on the variation over the full wavelength range and mostly reflects changing weather conditions. The flagging is oindicating the variability and this is not given in the standard colour scheme. The variability is given as the relative standard devation (in per cent) of the transmissions at the various wavewlengths.

Transmission 1 refers to the wavelength range from 300 –325 nm. The transmission is calculated but not flagged in view of the uncertainty of this transmission which depending strongly on the ozone estimate. The modelling is not regarded accurate enough to flag on this in the present version of SHIC.

The local shape flag indicates the variability of the ratiuo of two subsequent irradiance readings, compard to a similar ratio in the modelled spectrum. Together with teh spike-flag this is used to identify local deviations in the spectral structure. This flag is sensistive to very rapid changes in environmental conditions but not in slow variations during the scan.

```
1280900  2002  sza   49.213 UVA_transmission: GREEN  THICK_CLOUDS          scan_variability:
                    CONSIDERABLE_VARIATION_SCAN    local: GREEN STABLE  indicative eff. ozone:   300.58 DU
shift1_flagging          GREEN                  0.055 (nm)
shift2_flagging          GREEN                  0.039 (nm)
start_irradiance_flag    GREEN                  0.0000002 maximum_below_first:  0.0000001
Spike+local_shape        GREEN
Transmission_2           GREEN  THICK_CLOUDS          0.17835787  12.23   all 0.18388002  13.86
scan_variability_2       CONSIDERABLE_VARIATION_SCAN    12.23 =sd trans2
Transmission_1           NOT_IMPLEMENTED             0.20000471  14.33
local_shape_flag         GREEN STABLE              2.28 % criterium and nr_spikes   0.250      0    0.500      0    5.000      0
spike_flag_median_based  GREEN   nr_spikes_above_irr:     0.00050000     0 nr_spikes_above_irr0:     0.00010000     0
                                                                                    detected:     0
start_wavelength_flag            GREEN                  293.09 (nm)   efuv_below:   0.00 %
last_wavelength_flag             GREEN                  400.00 (nm)   efuv_above:   0.00 %
Median_irradiance_flag           NOT_EXTREME                Median_Irradiance:     0.01200355 at 310.00 nm
```

4.2 Corrected spectral irradiance

NORMALIZED AND CORRECTED SPECTRAL UV-IRRADIANCE

The directory NLR itself will have output files with standardised spectral output. For the example given above: 1621030i.NLR, where i is the id_specout identifier for the analysed standardised spectral irradiance. This file includes two shift corrected spectral irradiance columns with 0.5 nm wavelength steps. The two irradiance columns correspond to two slit functions:

- a standard slit (usually triangular slit with a FWHM of 1.0 nm) and
- the slit function provided for the instrument.

The normalised and corrected spectra extend up to 400 nm (or higher if specified in settings, maximum 600 nm), even if the instrument does not measure up to 400 nm. If the upper wavelength limit of the measurement is exceeded the program adds a note tot the data line: !NOTE: above measured wavelength.

4.3 Wavelength shift results

RESULTS OF WAVELENGTH SHIFT ANALYSIS

The subdirectory NLR\SHIFT\ contains the results for the analysed spectral shifts in three types of output-files:

- 1621030s.NLR, where 's' equals the id_shift, contains the detailed information on the shift analysis; wavelength interval for the shift determination, the shift and an estimated uncertainty in the shift, and the error ratio (shape error = ER) is provided. If the error ratio (ER) exceeds the smallest of 0.06, and 3.5 times the minimal value for the ER the message "!Error Ratio exceeds:" appears on the data line, and the shift result is not used in the deconvolution analysis. Furthermore the significance of the wavelength fit is estimated and if the fit is not significant at 1% the remark NOT_SIGNIFICANT is added to the dataline and also these shifts are not used. In case of too large errors or non-significant shifts the shift is then obtained interpolating (or extrapolating) from closest shift determinations that do not exceed the upper limit for the ER. If no shift is found to be reliable the shift used in the anlysis is 0 nm.
- 1621030w.NLR, where 'w' equals the id_shif_appl, provides two columns: the measured wavelength and the shift applied for that wavelength. Results are derived from the detailed shift results in the 's'-files.
- 162shis.NLR, provides daily variation in the wavelength shifts for all spectra of a day. Results for a subset of wavelength intervals are provided.

A summary of shift results per spectrum is given in the files 162QC.NLR, which are placed in the NLR\QAQC\ subdirectory (see section Summary of wavelength shift and anomaly analysis, below).

4.4 Effective UV calculation results

RESULTS OF EFFECTIVE UV AND INTEGRATED IRRADIANCE

The subdirectory NLR\EFUV\ contains result files with effective UV irradiances based on the shift corrected and deconvoluted data files. Several action spectra are used and wavelengths are integrated up to 325, 350, 365 and 400 nm. Filenames (for day 162): 162ef325.NLR, 162ef350.NLR etc. Furthermore analysed irradiance data are provided for certain wavelength ranges: 162_step.NLR

4.5 Summary QA/QC spike analysis

RESULTS OF SPECTRAL ANOMALY ANALYSIS

The subdirectory NLR\QAQC\ provides information on all flags for all analysed data, details on strucutural errors and on the main flagging parameters for all spectra, brougth together in daily files:

DDDQflag.LLL	contains all quality flagging information
DDDQC.LLL	contains summarising flag-parameters that determine all flags
DDDstr01.LLL	local structural shape errors (distortions) at 10% relative error
DDDstr25.LLL	local structural shape errors (distortions) at 25% relative error (this is used for the determination of the start irraidance flag)
DDDstr05.LLL	local structural shape errors (distortions) at 50% relative error
DDDstr5.LLL	local structural shape errors (distortions) at 500% relative error

The data on structural checks for the analysed spectra, which can be useful in identifying unexpected spectral anomalies in the shape of the spectrum, are derived from the ratio of spectral irradiances and are determined for all readings at successive wavelength pairs. This measured ratio is compared with the expected theoretical ratio obtained from the Extra-terrestrial spectrum in combination with the ozone absorption. Large spectral anomalies are reported in daily files that contain the anomalies exceeding certain limits for each individual spectrum. If a spectral name is followed by a blank line no anomalies exceeding the particular limit is found. Four levels of anomalies are reported in separate files (example-names for day 162 of instrmnet NLR: 162str01.NLR; 162str25.NLR, 162str05.NLR and 162str5.NLR).

The files that contain str01 report anomalies that exceed a factor of 1.10 (10%), str25 those that exceed 1.25 (25%), str05 those that exceed a factor of 1.5 (50%), and str5 those that exceed a factor of 6 (500%). It should be noted that the shift analysis and deconvolution are based on all data as provided in the data file, including those wavelengths which are reported with (possible) spectral anomalies.

5 REFERENCES

H.Slaper, T. Koskela Methodology of intercomparing spectral sky measurements, correcting for wavelength shifts, slit function differences and defining a spectral reference; in B. Kjeldstad, B.Johnsen, T Koskela (eds.) The Nordic intercomparison of ultraviolet and total ozone instruments at Izana in October 1996. Final report, Finnish Meteorological Institute, Meteorological Publication No 36, 89-108, ISBN 951-697-475-9, Helsinki, 1997.

H. Slaper methods for intercomparing instruments, chapter 2B in AR Webb (Ed) Advances in solar ultraviolet spectroradiometry, 153-164, Air Pollution Research Report EUR 17768, 1997.

H. Slaper, HAJM Reinen, M Blumthaler, M. Huber, F Kuik, Comparing ground level spectrally resolved solar UV measurements using various instruments: A technique resolving effects of wavelength shift and slit width, Geophys. Res. Lett. 22, 2721-2724, 1995.

Extra terrestrial spectrum based on a combination of data from the Kitt Peak Observatory (NSO/Kitt Peak FTS data used here were produced by NSF/NOAO) and Atlas 3

Ozone cross sections used are derived from:
Bass and Paur (1984) Proceedings of the Quadrennial ozone symposium, Halkidiki, Greece, 606-610, 1984.