# GOTOCORD

GOME Total Ozone Column Retrieval Development:

ESA ITT AO/1-4235/02/I-LG
ESRIN/Contract No. 16402/02/I-LG

## WFDOAS Software User Document

Issue 1.0

M. Coldewey-Egbers, M. Weber, and L.N. Lamsal

Institute of Environmental Physics, University of Bremen

Address:
Institute of Environmental Physics
Institute of Remote Sensing
University of Bremen FB1
P.O. Box 330 440
D-28334 Bremen
Germany

Contact:
Mark.Weber@uni-bremen.de


October 2004

# Contents

# Chapter 1

# Introduction

This document decribes the WFDOAS (Weighting Function Differential Optical Absorption Spectroscopy) algorithm software for UNIX workstations to retrieve total ozone in the Huggins band from GOME UV spectral data (Coldewey-Egbers *et al.*, 2003, 2004), including the main fitting program `kvant`, the preparation of GOME data for the fit, the FRESCO cloud algorithm of Koelemeijer *et al.* (2001), and the calculation of the reference and Ring data base.

The WFDOAS software has been developed at the Institute of Environmental Physics (IUP), University of Bremen, Germany, as part of the ESA/ESRIN contract 16402/02/I-LG.

The main fitting program is based on the WFM–DOAS (Weighting Function Modified – DOAS) algorithm, which has been developed by M. Buchwitz (Buchwitz *et al.*, 2000) for trace gas column retrieval in the near infrared region of SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography).

The results of an extensive pole-to-pole validation of the WFDOAS ozone algorithm for GOME with ground based data can be found in Weber *et al.* (2004a,b,c).

## 1.1 Installation

The current set-up for WFDOAS V1.0 including all look-up-tables can be foound on three DVDs. All directories under

`/wfdoas`

have to be copied from DVD. The entire dataset also includes FRESCO output for all GOME orbits from June 1995 until June 2003 and is distributed over three DVDs. All programs (`fresco` and `kvant`) have been tested for AIX, SOLARIS, and LINUX operation sytems. Programs written in fortran were compiled on LINUX using the ifc fortran compiler (http://developer.intel.com/software/products/global/eval.htm).

In order to access the databases the following files have to be de-archived:

```
/wfdoas/Version1/HIGH_LAT.tar
/wfdoas/Version1/MID_LAT.tar
/wfdoas/Version1/LOW_LAT.tar
/wfdoas/fresco_update/data.tar
```

Files contained in `data.tar` have to be gunzipped after the de-archiving. Specific compilation instructions for the various programs are given in the following sections.

## 1.2 Syntax of this document

Text in `typewriter style` denotes program and script names, variables, or directories and has to be written verbatim. *Slanted roman text* denotes a symbolic name for which a value has to be inserted. A vertical bar | separates two or more items in a list, from which exactly one has to be selected.

## 1.3 How to use WFDOAS

For total ozone retrieval from GOME data, two steps are required. First, the GOME level 1 data have to be prepared for the fit using the so-called extraction software `gome2mea_orbit_v6`, and second the retrieval itself using the `kvant` program.

It is not necessary to change anything concerning the reference and Ring data base, which are included in our software package. Also the FRESCO cloud information is available until June 2003.

### 1.3.1 Prepare GOME data for the fit

To prepare the GOME data for the fit, call the shell script

```
/wfdoas/sh/gome2mea_orbit_v6.sh ASC|HDF orbit.list
```

from any directory. Select between ascii (`ASC`) and `HDF` output. Note that the HDF output needs only 70% (about 6.5 MByte for one orbit) of the disk space compared to the ascii output (≈ 9 MByte). On the other hand, computation time is prolonged by a factor of 5 for the HDF format (1 minute for the ascii format and 5 minutes for the HDF format). The file `orbit.list` (any name can be used) is a list of orbits and pixels, which are to be extracted. The syntax of `orbit.list` is:

```
70915171            → Entire orbit 70915171 will be extracted
70915084 100 200    → Extract pixels number 100 to 200 of orbit 70915084
60102086 123        → Extract pixel number 123 of orbit 60102086
```

The different output files (radiance `radp_*` and irradiance `solp_*` in ascii (file extension `.mea`) or HDF format (file extension `.h5`), which are required for `kvant`, will be created in the current directory. Additionally, a log file is created, which contains the information if the extraction was successful.

Make sure, that the GOME level 1 data are stored in separate directories as described in Section 1.6.

FRESCO data, which are needed by the extraction software to obtain the ghost vertical column, are available from June 1995 to June 2003 and stored in the directory `/wfdoas/fresco_update/data`. If you would like to prepare GOME data past June 2003, first use the script

```
/wfdoas/sh/O2Aextract_fresco.sh
```

to retrieve the cloud information from GOME. Then proceed with the extraction software.

For a detailed description of the extraction software and FRESCO, see Chapters 2 and 3.2, respectively.

### 1.3.2 `kvant` ozone fitting program

The shell script

`/wfdoas/sh/kvant.sh`

starts the execution of the kvant program. Call:

`/wfdoas/sh/kvant.sh` *radp_orbit_pixel0_pixel1 outname* `or|nr V1 HDF|ASC SOL|NOSOL`

| | |
|---|---|
| *radp_orbit_pixel0_pixel1* | → The radiance file, must be in the current directory. |
| *outname* | → Tag for outputfile(s) |
| `or|nr` | → Select between old and new Ring version |
| `V1` | → Version (`V1` only at the moment) |
| `HDF|ASC` | → Select input and output format, HDF or ascii, must be the same as for the extraction. |
| `SOL|NOSOL` | → `SOL`: solar spectrum from database<br>`NOSOL`: solar spectrum from *.lv1 file (`solp_*` file) |

Please note, the combination *HDF* and *SOL* is not allowed, as the external solar database, which is stored in the directory

`/wfdoas/solar/`,

is in ascii format only.

The shell script `kvant.sh` creates the configuration file `kvant.cfg` and starts the execution of `kvant`. See Section 6.2 for a detailed description of the keywords in `kvant.cfg`. Both main and extended output files are created in the current directory. See Section 6.5 for a detailed description of the content of the output files.

## 1.4 Theory of WFDOAS

The measured atmospheric optical depth is approximated by a Taylor expansion around the reference intensity plu a low-order polynomial. The total column information is obtained only from differential trace gas absorption structures. The cubic polynomial accounts for all broadband contributions such as surface albedo and aerosol. The optical depth equation can be written as follows:

$$\begin{aligned}
\ln I_i^{mea}(V^t, \vec{b}^t) \approx\ & \ln I_i^{mod}(\bar{V}, \bar{\vec{b}}) \\
& + \frac{\partial \ln I_i^{mod}}{\partial V}|_{\bar{V}} \times (\hat{V} - \bar{V}) \\
& + \frac{\partial \ln I_i^{mod}}{\partial T}|_{\bar{T}} \times (\hat{T} - \bar{T}) \\
& + SCD_{NO_2} \cdot \sigma_{i,NO_2} \\
& + SCD_{BrO} \cdot \sigma_{i,BrO} \\
& + SCD_{Ring} \cdot \sigma_{i,Ring} \\
& + SCD_{usamp} \cdot \sigma_{i,usamp} \\
& + P_i
\end{aligned} \tag{1.4.1}$$

$I^{mea}$ is the measured intensity and $I^{mod}$ the sun-normalized reference intensity as provided by the radiative transfer model. Index $t$ denotes the true atmospheric state. The entire right-hand side of the equation (excluding the reference intensity) has to be adjusted to the measured intensity (left-hand side) for all spectral points (index $i$) simultaneously. $\bar{V}$ is the reference ozone column corresponding to the reference intensity, and $\bar{T}$ is the

Table 1.4.1: *Parameter space of the look-up-tables. (*) min/max of relative azimuth angle depend on SZA and LOS.*

| Atmospheric Parameter | Min | Max | $\Delta$ | N |
|---|---|---|---|---|
| Total Ozone (high latitudes) | 125 DU | 575 DU | 50 DU | 10 |
| Total Ozone (mid latitudes) | 125 DU | 575 DU | 50 DU | 10 |
| Total Ozone (low latitudes) | 225 DU | 475 DU | 50 DU | 6 |
| Solar Zenith Angle | 15° | 92° | 5° if SZA $\leq$ 70°<br>1° if SZA $>$ 70° | 34 |
| Line-Of-Sight | -34.5° | 34.5° | 11.5° | 7 |
| Relative Azimuth Angle | (*) | (*) | | 3 |
| Surface Albedo | 0.02 | 0.98 | $\sim$ 0.2 | 6 |
| Altitude | 0 km | 12 km | 2 km | 7 |

reference surface temperature. $\hat{V}$ and $\hat{T}$ denote the corresponding fit parameters. The Ring effect ($\sigma_{i,Ring}$) and the under-sampling spectrum ($\sigma_{i,usamp}$) (Slijkhuis *et al.*, 1999) are treated as effective absorbers similar to the approach used in standard DOAS. Slant column fitting is also applied to the minor absorbers $NO_2$ and BrO. The unknown fit parameters are derived using a linear least squares minimization. The retrieved scalar temperature correction $\Delta T = \hat{T} - \bar{T}$ actually represents a shift in the entire vertical temperature profile. It accounts for the dependence of the observed ozone absorption on stratospheric temperature.

The main difference between the WFDOAS algorithm and the standard DOAS is the use of wavelength dependent weighting functions instead of absorption cross-sections and airmass factors. Weighting functions describe the relative radiance change due to a vertical profile change assuming an altitude independent scaling factor.

A large set of reference spectra has been constructed, which includes nearly all possible atmospheric conditions. The radiance spectra and weighting functions are computed as a function of total ozone including profile shape, solar zenith angle, line-of-sight, relative azimuth angle, surface albedo, and altitude. See chapter 4 for a detailed description, how the reference data base has been generated.

Table 1.4.1 gives an overview of the parameter space. Ozone and temperature profiles are taken from TOMS V7 (Total Ozone Mapping Spectrometer Version 7) climatology (Wellemeyer *et al.*, 1997) which contains different profile shapes for three latitude belts (low, middle and high) as a function of the total ozone column. The dependence of the relative azimuth angle on solar zenith angle and line-of-sight has been obtained using all GOME orbits from 1998. The minimum, maximum, and mean angles are taken for reference spectra calculation for a given combination of solar zenith angle and line-of-sight. Altitude of the boundary in the lower atmosphere varies between 0 and 12 km. In the actual retrieval this altitude is identified with the effective height derived from the GOME scene (see Section )

All reference spectra have been computed with the SCIATRAN/CDI code, an extension of the GOMETRAN++ radiative transfer model (Rozanov *et al.*, 1997, 1998) in the pseudo-spherical approximation. It was specifically developed for simulation of back-scattered intensities and is based on the finite differences approach. The viewing angles line-of-sight and solar zenith angle are taken at the ground level for this computation. Compared to the full spherical mode, the ground level viewing geometry (line-of-sight, solar zenith angle and relative azimuth) rather than top-of-atmosphere viewing geometry to be used in the pseudo-spheric approximation leads to lower slant column errors (de Beek *et al.*, 2004).

The shift and squeeze operation to improve the wavelength misregistration between the different spectra is limited to the earthshine spectrum, which is fitted to the GOME solar spectrum. Following the recommendation of Roozendael *et al.* (2003), a constant shift of +0.017 nm has been applied to GOME FM cross sections for ozone and nitrogen dioxide (Burrows *et al.*, 1998, 1999) before the calculation of reference spectra and weighting functions. In order to correct for the Doppler shift (+0.008 nm) in the solar reference and for wavelength calibration errors using the onboard Pt/Ne/Cr hallow cathode lamp, the GOME solar spectrum is nonlinearly fitted to a high resolution solar atlas derived from Fourier transform spectrometer measurements carried out with

the McMath Solar Telescope, Kitt Peak Observatory, Arizona (Kurucz *et al.*, 1984). This so-called Fraunhofer fitting is done before the DOAS fit is performed.

We selected the 8.2 nm wide fit window from 326.8 - 335.0 nm for ozone retrieval. In case of cloud contaminated ground pixels, the part of the ozone column, which is below the top of the clouds, cannot be detected by the satellite. This ghost vertical column (GVC) has to be estimated from climatological vertical ozone profiles and is added to the vertical column retrieved from the spectral fit. The GVC is computed by integrating the profile from surface pressure up to the cloud top pressure. Partial cloudiness can be taken into account by multiplying the integrated column with fractional cloud cover from FRESCO (Fast Retrieval Scheme for Clouds from the Oxygen A-Band) (Koelemeijer *et al.*, 2001) as follows:

$$GVC = f \cdot \int_{h'=h_o}^{h_{cld}} [\mathsf{O}_3(h')]\, dh'. \tag{1.4.2}$$

$f$ and $h_{cld}$ are the fractional cloud cover and cloud-top-height retrieved with FRESCO, respectively. $h_o$ is the surface height of the GOME scene and $[\mathsf{O}_3(h)]$ the ozone concentration at altitude $h$. For the integration of the tropospheric column up to the cloud-top-pressure, ozone profiles from the TOMS V8 monthly and zonal mean climatology (G. Labow, private communication) are used. This climatology was compiled from ozone sonde data, SAGE II, and POAM III satellite data in the 90s (G. Labow, private communication). The latter climatology takes hemispherical (ten degree latitude steps) and seasonal differences (monthly mean) into account. The TOMS V7 climatology as used for the reference scenario and weighting functions provides a better representation of the stratospheric variability but is not as well suited for a tropospheric climatology. Figure 1.4.1 shows the schematics of the GVC determination.

Chapter 3 gives a description of the FRESCO algorithm and the program output, which is needed for preparing GOME data for the `kvant` ozone fitting algorithm.

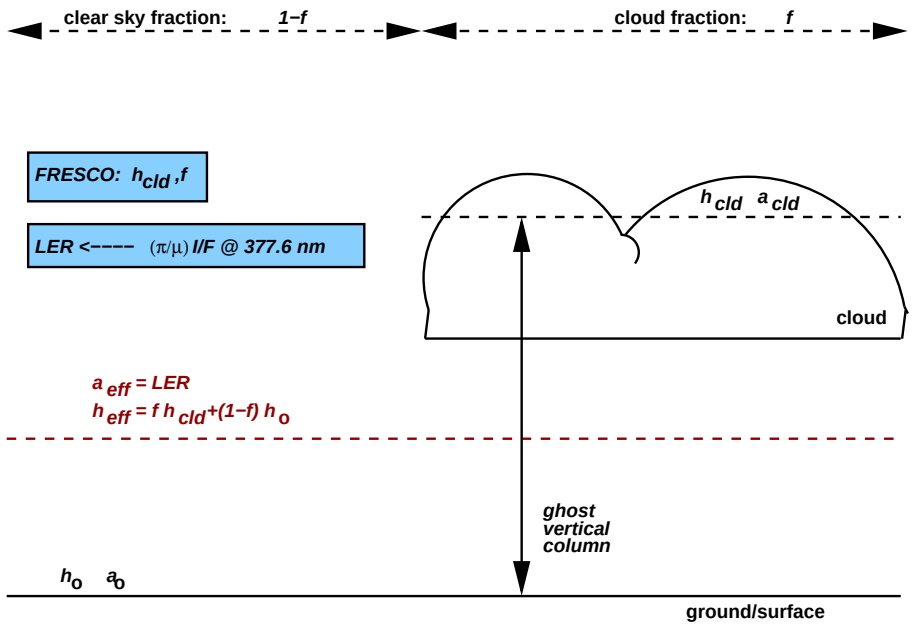


Figure 1.4.1: *Definition of various parameters defined for cloud retrieval from GOME using FRESCO (Koelemeijer* et al.*, 2001) and the ozone ghost vertical column correction. Cloud fraction $f$ and cloud top height $h_{cld}$ are retrieved from the oxygen A2 band absorption assuming a constant cloud albedo ($a_{cld} = 0.8$). Surface albedo $a_o$ near 760 nm is taken from a 5-year GOME database (Koelemeijer* et al.*, 2001). The effective UV albedo $a_{eff}$ is determined using the Lambertian equivalent reflectivity approach near 377 nm (see text). The effective scene height $h_{eff}$ is then calculated from the weighted average of cloud-top-height $h_{cld}$ and surface height $h_o$ weighted by the cloud fraction ($h_{eff} = f \cdot h_{cld} + (1 - f) \cdot h_o$). The ghost vertical column (GVC) is determined by integrating a climatological profile from surface to the retrieved cloud-top-height and then multiplying the integrated sub-column by the cloud fraction (see text for details).*

## 1.5 Directory structure

This section gives an overview of the directory structure used for WFDOAS. Not included in this structure is the storage of the GOME level 1 data (see following section 1.6), and the generation of the reference and Ring data base (see chapters 4 and 5).

```
wfdoas
|
|
|------ sh → Contains all shell scripts
|
|
|------ extraction
|       |
|       |------ aux → Contains the program to prepare of GOME data for the fit
|
|
|------ fresco_update
|       |
|       |------ data → Contains FRESCO output
|       |------ bin → Contains FRESCO software
|
|
|------ Version1
        |
        |------ kvant_auxinput → DOAS spectra (NO2, BrO, undersampling, old Ring)
        |
        |------ program
        |       |
        |       |------ f90
        |       |       |
        |       |       |------ programs → Main program kvant.f90
        |       |       |------ make → Makefile to compile the program
        |       |       |------ modules → Modules for kvant.f90
        |       |
        |       |------ bin → kvant executable
        |
        |------ HIGH_LAT
        |       |
        |       |------ subdirectories see LOW_LAT
        |
        |------ MID_LAT
        |       |
        |       |------ subdirectories see LOW_LAT
        |
        |------ LOW_LAT → Reference spectra for 20 different scan modes
        |                 → and Ring spectra for low latitudes
                |
                |------ MeanEastBinary
                |------ MeanNadirBinary
                |------ MeanWestBinary
                |------ BackScanBinary
                |------ FullScanBinary
                |
                |------ SmallScanEastBinary
```

```
|——— SmallScanNadirBinary
|——— SmallScanWestBinary
|——— SmallScanBackScanBinary
|——— SmallScanFullScanBinary
|
|——— NoCoaddEastBinary
|——— NoCoaddNadirBinary
|——— NoCoaddWestBinary
|——— NoCoaddBackBinary
|
|——— StaticScanBinary
|
|——— TestScanEastBinary
|——— TestScanNadirBinary
|——— TestScanWestBinary
|——— TestScanBackScanBinary
|——— TestScanFullScanBinary
|
|——— RING
```

## 1.6 Storage of GOME Level 1 Data

The GOME Level 1 data are not included in our software package. They have to be stored in separate directories of the following structure:

`/GOME_LVL10/`*year/month/day/orbit*`.lv1`.

`/GOME_LVL10/` must be parallel to `/wfdoas/`.

# Chapter 2

# Preparation of GOME data for kvant

The program /wfdoas/extraction/aux/gome2mea_orbit_v6.f prepares GOME data for the ozone retrieval with kvant. The program, routines, input files, and shell scripts are in the subdirectory

/wfdoas/extraction/aux/.

The following files are needed to prepare the GOME data:

- Programs and scripts

  | | |
  |---|---|
  | gome2mea_orbit_v6.f | → Main program |
  | gome2mea_orbit_v6_ASC.x | → Executable (format ascii on SUN platform) |
  | gome2mea_orbit_v6_HDF.x | → Executable (format HDF on SUN platform) |
  | gome2mea_orbit_v6_ASC.lx | → Executable (format ascii on linux platform) |
  | gome2mea_orbit_v6_HDF.lx | → Executable (format HDF on linux platform) |
  | write_extrt_hdf5.f90 | → Create output in HDF format |
  | gomemea_check_list.sh | → |
  | lv1_extract.sh | → GOME level 1 extraction |

- Input files

  | | |
  |---|---|
  | gome_orbit_list.txt | → List of orbits and pixels to be processed |
  | glo3-final.dat | → TOMS V8 Climatology |
  | guzzi_hgt_1x1.dat | → Guzzi altitude data base |
  | ler_t3.bin | → TOA radiances for LER retrieval |

- Output files

  | | |
  |---|---|
  | radp_*orbit*.mea | → Radiance and auxiliary information in ASCII format |
  | radp_*orbit*.h5 | → Radiance and auxiliary information in HDF format |
  | solp_*orbit*.mea | → Solar irradiance in ASCII format |
  | solp_*orbit*.h5 | → Solar irradiance in HDF format |

## 2.1 Running the program

For running the program in any directory, call the shell script

```
/wfdoas/sh/gome2mea_orbit_v6.sh ASC|HDF orbit.list
```

Select between ascii (`ASC`) and `HDF` output. The file `orbit.list` (any name can be used) is a list of orbits and pixels, which are to be extracted. The syntax is:

```
70915171           → Entire orbit 70915171 will be extracted
70915084 100 200   → Extract pixels number 100 to 200 of orbit 70915084
60102086 123       → Extract pixel number 123 of orbit 60102086
```

The different output files with radiance and irradiance in ascii or HDF format as described above will be created in the current directory. Additionally, a log file is created.

### 2.1.1 Process an entire month

For easily processing a whole month call the shell script:

```
/wfdoas/sh/gome_orbit_extract.sh ASC|HDF ''907*''
```

This script calls the script `gome2mea_orbit_v6.sh` for all orbits of July 1997, for example.

### 2.1.2 Example output files

The ASCII radiance file `radp_`*orbit*`.mea`:

```
'*NEW*' 0.0              → New Pixel
'*DAY:' 19960612         → Date: 06 Dec 1996
'*TIM:' 35899392.        → Time: Milliseconds after launch
'*PIX:' 867              → Pixel number
'*SUB:' 2                → Subpixel counter: west
'*SCM:' no_w             → Scan mode: normal west pixel
'*SZA:' 29.67            → Solar zenith angle [°]
'*LOS:' 22.35            → Line-of-sight [°]
'*AZI:' 133.25           → Relative azimuth angle [°]
'*GRD:' 1.59             → Effective altitude [km]
'*LA1:'  49.86           → Latitude of first pixel corner [°]
'*LA2:'  50.20           → Latitude of second pixel corner [°]
'*LA3:'  50.39           → Latitude of third pixel corner [°]
'*LA4:'  50.80           → Latitude of fourth pixel corner [°]
'*LAT:' 50.30            → Latitude of pixel center [°]
'*LO1:'  16.11           → Longitude of first pixel corner [°]
'*LO2:'  16.24           → Longitude of second pixel corner [°]
'*LO3:'  11.48           → Longitude of third pixel corner [°]
'*LO4:'  11.60           → Longitude of fourth pixel corner [°]
'*LON:' 14.16            → Longitude of pixel center [°]
'*CF_:'  0.25            → Cloud fraction
'*H_0:'  0.29            → Surface altitude [km]
'*H_C:' 5.43             → Cloud top height [km]
'*GVC:' 4.96             → Ghost vertical column [DU]
'*CO3:'  0.9111635D+19   → Initial ozone column [molec/cm^2]
'*CNO:' 0.3247000D+16    → Climatological NO2 Column [molec/cm^2]
'*CBR:' 0.2000000D+14    → Climatological BrO Column [molec/cm^2]
'*PRE:' 0.1013000D+04    → Surface Pressure [hPa]
'*TEM:' 0.2880000D+03    → Surface Temperature [K]
'*ALB:' 0.2735150D+00    → LER
'*NSP:' 174              → Number of spectral points
320.2212 .1044980D+14    → Wavelength [nm] and Radiance []
320.3365 .1123070D+14    →
320.4517 .1255530D+14
...
...
...
339.7347 .2015700D+14
339.8478 .2154030D+14
339.9609 .2151720D+14
'*NEW*' 0.0              → Second pixel
'*DAY:' 19960612
'*TIM:' 35900892.
⋮
```

The ASCII irradiance file `solp_`*orbit*`.mea`:

```
'*NSP:' 165              → Number of spectral points
320.1060 .1277470D+15    → Wavelength [nm] and irradiance []
320.2212 .1279120D+15
320.3365 .1329380D+15
...
...
...
338.6035 .1722390D+15
338.7166 .1872940D+15
338.8298 .1612620D+15
⋮
```

## 2.2 Program structure `gome2mea_orbit_v6`

1. Read the GSFC Climatology (TOMS V8). It contains the temperature, pressure, air density, and ozone volume mixing ratio (VMR) as a function of month (January to December), altitude (0–60 km in steps of 300 m), and zonal band (90–80°S, ..., 80-90°N). The Ozone VMR is then converted into number density.

2. Read the altitude data base from Guzzi `guzzi_hgt1x1.dat` with subroutine `guzzi_table()`. It provides terrain height information [m] on a 1x1 degree grid.

3. Read the table `ler_t3.bin` which contains top-of-atmosphere radiances as a function of altitude, line-of-sight, relative azimuth angle, solar zenith angle, and surface albedo at 377.6 nm for LER retrieval with subroutine `tabledata_L3_new()`.

4. Read the list of orbits and pixels to be processed from the file `gome_orbit_list.txt`. Following entries are possible:

   ```
   70915171           → Process the whole orbit
   70915171 150 200   → Process pixels 150 to 200
   70915171 150       → Process only pixel number 150
   ```

5. Run the shell script `gomemea_check_list.sh` to check whether all orbits and pixels (GOME level 1 data) are available.

6. Read the FRESCO cloud information with the subroutine `ReadFresco()` from separate data base, that can be found in the directories

   `/wfdoas/fresco_update/data/`*year/month/*.

   In case of FRESCO's normal mode, cloud top pressure, surface pressure, and cloud fraction are extracted. In case of FRESCO's snow and ice mode, the effective reflectivity and pressure of the effective altitude are extracted.

7. Calculate the effective altitude using the subroutine `CalcEffHgt()`. First, cloud top pressure and surface pressure are converted into altitudes [m] using the US Standard Atmosphere. The calculation of the effective altitude follows the assumption that

   $$\mathrm{ehgt} = \mathrm{cth} \cdot \mathrm{cf} + \mathrm{sh} \cdot (1 - \mathrm{cf}),$$

   where ehgt is the effective height, cth is the cloud top height, cf is the cloud fraction, and sh is the surface height. In case of FRESCO's snow and ice mode, only the pressure of the effective height has to be converted into an altitude.

8. Extract GOME level 1 data using the shell script `lv1_extract.sh`. File *orbit*`.el1` is created.

9. Open the output files for radiance and irradiance information

   `radp_`*orbit*`.mea` and `solp_`*orbit*`.mea`
   or
   `radp_`*orbit*`.h5` and `solp_`*orbit*`.h5`

10. Read GOME level 1 data from *orbit*`.el1` file.

    (a) Read solar data (channel 2 only)

    (b) Read radiance data (channel2 only)

    (c) Check which pixel type (0.375, 1.5, or 6 sec integration time)

(d) Get measurement day and time

(e) Extract viewing geometry at satellite altitude

(f) Calculate viewing angles at TOA using the subroutine `angles()`

(g) Calculate the surface altitude, a weighted sum of 4 pixel corners and the pixel center

(h) Retrieve the Lambert Equivalent Reflectivity (LER) from GOME sun-normalized radiance at 377.6 nm, where the variation with respect to the Ring effect can easily be corrected. The viewing geometries are taken from GOME observations, altitude input is the effective altitude from FRESCO (see item No. 7). For this set of parameters , radiances as a function of albedo are extracted from the table (see item No. 3). The LER is obtained by a bi-sectional search along this curve.
Subroutines `spline()`, `splint()`, and `multilin_l3_new()` are used.
If the retrieved LER is below 0.02, it is set to 0.02, and if it is above 0.98, it is set to 0.98. Otherwise, the LER will be out of the parameter space of the kvant reference and Ring data bases.

(i) Determine the scan mode. The following scan modes exist:

| Mode | Line-of-sight | Tag for scanmode | Integration time [sec] |
|---|---|---|---|
| Normal | east | no_e | 1.5 |
| Normal | nadir | no_n | 1.5 |
| Normal | west | no_w | 1.5 |
| Normal | backscan | no_b | 1.5 |
| Normal | fullscan | no_f | 6.0 |
| Small swath width | east | ss_e | 1.5 |
| Small swath width | nadir | ss_n | 1.5 |
| Small swath width | west | ss_w | 1.5 |
| Small swath width | backscan | ss_b | 1.5 |
| Small swath width | fullscan | ss_f | 6.0 |
| NoCoadd | east | nf_e | 0.375 |
| NoCoadd | nadir | nf_n | 0.375 |
| NoCoadd | west | nf_w | 0.375 |
| NoCoadd | backscan | nf_b | 0.375 |
| Static scan | nadir | stat | 1.5 |
| Test scan | east | te_e | 1.5 |
| Test scan | nadir | te_n | 1.5 |
| Test scan | west | te_w | 1.5 |
| Test scan | backscan | te_b | 1.5 |
| Test scan | fullscan | te_f | 6.0 |

(j) Calculate initial ozone value from TOMS V8 climatology. Input data are month and zonal band.

(k) Calculate the ghost vertical column (GVC) using the FRESCO cloud information and the TOMS V8 ozone profile climatology.

(l) Create radiance output file. All pixels of one orbit are together in one file. The wavelength window is restricted to 320 to 340 nm.

(m) Create the solar output file (one file for each orbit).

11. Proceed with the next line of `gome_orbit_list.txt`

# Chapter 3

# FRESCO

## 3.1 Algorithm description

This section contains a short description of the Fast Retrieval Scheme for Clouds from the Oxygen A-band (FRESCO algorithm), which is used to obtain the ghost vertical columns from GOME data. A detailed description can be found in Koelemeijer *et al.* (2001).

### 3.1.1 Principle

The algorithm has been developed to retrieve the effective cloud fraction and cloud top pressure from GOME data. The algorithm uses reflectivities measured by GOME inside and outside the oxygen A-band from 758 - 778 nm. The reflectivities are normalized by their continuum value at 758 nm, where no absorption occurs. This value is mainly determined by the cloud fraction, the cloud optical thickness (or cloud albedo) and the surface albedo. Inside the oxygen A-band, the reflectivity depends on the cloud top pressure as well, because clouds screen nearly all the oxygen below them. Therefore the oxygen A-band is deeper for pixels with low clouds than for pixels with high clouds. Combined information on cloud fraction and cloud optical thickness may be derived from the reflectivity in the continuum, whereas the cloud top pressure can be inferred from the depth of the oxygen A-band, as oxygen is a well mixed gas.

For a detailed description see the FRESCO user guide, that can be found in

`/wfdoas/fresco_update/frug.pdf`.

### 3.1.2 Method description

The FRESCO software has two operation modes, depending whether the surface is assumed to be free of snow/ice or not. The first mode is refered to as the normal mode and the latter mode is the snow/ice mode.

1. Normal mode
   The effective cloud fraction is derived by assuming that the cloud is an elevated isotropically reflecting surface with an albedo of 0.8. The derived cloud top pressure is the pressure at this elevated surface. If the measured reflectivity outside the oxygen A-band is higher than 0.8, the effective cloud fraction is set to 1, and the cloud albedo is set to the reflectivity outside the band, i.e. higher than 0.8.
   The cloud top pressure becomes unreliable if the effective cloud fraction drops below 0.05. This is also indicated by the error on the retrieved cloud top pressure.

The effective cloud fraction assuming a cloud albedo of 0.8 pertains to a cloud with an optical thickness of 33, so that absorption below the cloud may be neglected. The surface height is taken from the ETOPO-5 database, downgraded to $1^\circ \times 1^\circ$ resolution.

2. Snow/ice mode
   If the surface is assumed to be covered by snow and ice, FRESCO cannot derive an effective cloud fraction, because this is basically determined from the contrast of the cloud with respect to the underlying surface. Therefore, what FRESCO derives in this mode is the pressure of the reflecting surface (reported in the cloud pressure column in the output file). The albedo of this reflecting surface is equal to the measured reflectivity outside the oxygen A-band (reported in the cloud albedo column). The reported effective cloud fraction is -1 in this mode.
   How is the snow/ice mode determined ?
   The global TOMS UV minimum surface reflectivity climatology, derived by Herman and Celarier (1997), is used for this. If according to this database the surface is brighter than 0.2 for a given month, it is assumed, that the surface is permanently covered by snow and ice. Then, the snow/ice mode is used, otherwise, the normal mode is used.

## 3.2 Compile and run the program

To compile the FRESCO program, use the makefiles `Makefile` for solaris and `Makefile_lx` for linux in the directory

`/wfdoas/fresco_update/bin/`

For running the program in any directory, call the shell script

`/wfdoas/sh/O2Aextract_fresco.sh ''907*''`,

which extracts all data from July 1997, for example, using the program `gdp01_ex_fresconeu`. The files *orbit*`_O2A.el1` are created, which contain the GOME level 1 data restricted to the wavelength range of the oxygen A-band (757–767 nm). Afterwards, the FRESCO program `fmain` is executed and the output files *orbit*`_fd.dat` are created and written in the directories

`/wfdoas/fresco_update/data/`*year/month/*.

### 3.2.1 Example output file

The FRESCO output file *orbit*`_fd.dat` contains the cloud and auxiliary information for each GOME pixel. The file has 15 header lines, reporting parameters in the `fresco.in` file.

Example output file:

```
# ==== FRESCO OUTPUT FILE ====
# instrument -- GOME (1) or SCIA (2) :  1
# cloud BRDF mode -- LAMBERT (0) or MIE_C1 (1) :  0
# max.  iterations in Levenberg Marquart fit :  5
# Lambertian cloud albedo (NOT used for MIE_C1) :  0.8000
# UV albedo threshold for snow/ice mode :  0.2000
# minimum surface albedo 758--772 nm :  0.0100
# first-guess effective cloud fraction :  0.5000
# first-guess cloud top height [km] :  5.0000
# first-guess cloud albedo :  0.5000
# Chi-square variation cut-off value :  0.10000E-04
```

```
# Error in simulated reflectivity :  0.10000E-01
# Maximum allowed solar zenith angle :  0.89500E+02
# Maximum allowed measured reflectivity :  0.12000E+03
# date time nr ss lat lon th th0 dphi c dc Pc dPc Ac dAc As ps chisq Q cov flag
19990708 190822 1 0 51.130 39.740 0.011 100.420 105.980 -1.000 -1.  000 -1.00 -1.00 -1.000
-1.000 -1.000 -1.00 -0.10000E+01 -0.10000E+01 -0 .10000E+01 2
19990708 191716 353 0 77.090 347.590 23.833 69.406 107.948 -1.000 -1.  000 919.62 32.00 0.381
0.005 0.000 1013.00 0.11778E+02 0.54590E+00 -0 .69855E-03 1
19990708 192215 552 3 75.680 263.530 1.347 53.749 113.659 0.277 0.  007 828.12 46.16 0.800
0.000 0.179 1012.18 0.73524E+01 0.88309E+00 -0 .15961E-02 0
⋮
```

The meaning of quantities in the columns defined in line 15 of the output file in the normal operation mode is: Notes give the meaning of the quantities in the snow/ice mode.

`date` → Aqusition time (YYYYMMDD)
`time` → Aqusition time (milliseconds have been truncated)
`nr` → Pixel number
`ss` → Subpixel counter
`lat` → Center latitude [deg] (range -90 to +90)
`lon` → Center longitude [deg] (range 0 to 360)
`th` → Viewing zenith angle at TOA [deg]
`th0` → Solar zenith angle at TOA [deg]
`dphi` → Azimuth difference angle between directions to sun and satellite at TOA [deg]
`c` → Effective cloud fraction (range 0 to 1), assuming cloud albedo `Ac`
→ Note: in snow/ice mode, `c` $= -1$
`dc` → Error in derived effective cloud fraction
`Pc` → Cloud top pressure [hPa]
→ Note: in snow/ice mode this is the pressure of the reflecting surface
`dPc` → Error in derived cloud top pressure
`Ac` → Assumed cloud albedo. Often, this will be 0.8, but may exceed 0.8,
→ if the measured reflectivity outside the oxygen A-band exceeds 0.8.
→ Note: in snow/ice mode, this is the albedo of the reflecting surface
`dAc` → Error on cloud albedo
`As` → Assumed surface albedo
→ Note: not used in snow/ice mode
`ps` → Assumed surface pressure
→ Note: not used in snow/ice mode
`chisq` → Chi-square fitting error
`Q` → Goodness-of-fit parameter
`cov` → Covaraince matrix element for fitted parameters
`flag` → Error flag [0,1,2,3,4,5]
→ `0`: default mode, fitting for `c` and `Pc`
→ `1`: snow/ice mode, fitting for `Ac` and `Pc`
→ `2-5`: FRESCO failure

# Chapter 4

# Reference database

This chapter contains the description how the reference data base has been established. For simply using the WFDOAS kvant software, no changes concerning the reference data base and the Ring data base (see following Chapter 5) are required.

A full set of reference spectra is already available.

In contrast to the main program `kvant` and the extraction software, which have been developed on Linux and SUN workstations, the reference and Ring data base have been computed on an IBM workstation.

## 4.1 Introduction

A large set of reference spectra has been constructed, which includes nearly all possible atmospheric conditions. The radiance spectra and weighting functions are computed as a function of total ozone including profile shape, solar zenith angle, line-of-sight, relative azimuth angle, surface albedo, and altitude.

Table 1.4.1 gives an overview of the selected parameter space. Ozone and temperature profiles are taken from TOMS V7 (Total Ozone Mapping Spectrometer Version 7) climatology (Wellemeyer *et al.*, 1997) which contains different profile shapes for three latitude belts (low, middle and high) as a function of the total ozone column. The dependence of the relative azimuth angle on solar zenith angle and line-of-sight has been obtained using all GOME orbits from 1998. The minimum, maximum, and mean angles are taken for reference spectra calculation for a given combination of solar zenith angle and line-of-sight. Altitude of the boundary in the lower atmosphere varies between 0 and 12 km.

Based upon this table and selected parameter space, the reference spectra have been computed using the radiative transfer code SCIATRAN (Rozanov *et al.*, 1997, 1998).

## 4.2 Create Reference Spectra

Based upon the table and parameter space described above, the reference spectra have been computed. The construction of the data base constists of several steps and programs, which have to be executed successively.

### 4.2.1 Directory structure

```
kvant_refspec
|
|------ HIGH_LAT
|       |
|       |------ subdirectories see LOW_LAT
|
|------ MID_LAT
|       |
|       |------ subdirectories see LOW_LAT
|
|------ LOW_LAT
        |
        |------ E1
        |------ E2
        |------ E3
        |------ N2
        |------ W1
        |------ W2
        |------ W3
        |
        |------ MeanEast
        |------ MeanNadir
        |------ MeanWest
        |------ MeanBackScan
        |
        |------ MeanEastBinary
        |------ MeanNadirBinary
        |------ MeanWestBinary
        |------ BackScanBinary
        |------ FullScanBinary
        |
        |------ SmallScanEastBinary
        |------ SmallScanNadirBinary
        |------ SmallScanWestBinary
        |------ SmallScanBackScanBinary
        |------ SmallScanFullScanBinary
        |
        |------ NoCoaddEastBinary
        |------ NoCoaddNadirBinary
        |------ NoCoaddWestBinary
        |------ NoCoaddBackBinary
        |
        |------ TestScanEastBinary
        |------ TestScanNadirBinary
        |------ TestScanWestBinary
        |------ TestScanBackScanBinary
        |------ TestScanFullScanBinary
        |
        |------ StaticScanBinary
```

All reference spectra are computed in each of the first seven subdirectories `E1, ..., W3` in each latitude directory `HIGH_LAT, MID_LAT,` and `LOW_LAT`.

Then the line-of-sight average is taken and the Chebyshev polynomials are computed. The final reference spectra, which contain only the polynomial coefficients for the LOS averaged spectra, are then written in 20 subdirectories `MeanEastBinary`, ..., `StaticScanBinary`. They define the 20 different scan modes and pixel types (see Section 2.2).

The four directories `MeanEast, ..., MeanBackScan` are used only for intermediate data storage.

### 4.2.2 Create control files for SCIATRAN

The following programs and script can be found in the uppermost directory `/kvant_refspec/`.

The program `write_controlfile.f` creates the shell script `write_controls.sh`, which calls the script `write_controlfile.sh`. As input for `write_controlfile.sh`, the file `control_dummy.inp` is needed. The parameters, which are varied for the different control files are

- total ozone
- latitude band for the TOMS V7 climatology (high, mid, or low)
- and altitude.

Important notice :
All other settings, which are needed to compute the reference data base, e.g. solar zenith angle, line-of-sigth, relative azimuth angle, and albedo, are defined later. The setting of these parameters in the control files, which are written using the `write_controlfile.sh` script, will be then replaced !

The control files are then named

`control_00`*xx*`00e`*y*`.inp.`*zzzz*, whereas

| | | |
|---|---|---|
| *xx* | → `01, ..., 10` | Total ozone index (`01` = 125DU, `02` = 175 DU, ..., `10` = 575 DU) |
| *y* | → `1, ..., 7` | Altitude index (`1` = 0 km, `2` = 2 km, ..., `7` = 12 km) |
| *zzzz* | → `lola, mila, hila` | Latitude index (`hila` = high latitude, `mila` = mid latitude, `lola` = low latitude) |

After having created all control-files, they have to be put in the beloning directories. That means, all `control*.hila` files have to be copied in each of the seven subdirectories

```
/HIGH_LAT/E1/control*.hila
/HIGH_LAT/E2/control*.hila
/HIGH_LAT/E3/control*.hila
/HIGH_LAT/N2/control*.hila
/HIGH_LAT/W1/control*.hila
/HIGH_LAT/W2/control*.hila
/HIGH_LAT/W3/control*.hila .
```

The same is valid for all `control*.mila` and `control*.lola` files, which have to be copied in the subdirectories of `/MID_LAT/` and `/LOW_LAT/`, respectively.

### 4.2.3 Create lists of reference spectra to be generated

Besides the control-files for SCIATRAN, also lists of all reference spectra, which are to be generated, have to be written. In the uppermost directory `/kvant_refspec/`, the program `write_refspeclisttxt.f`

(executable: `write_refspecliststxt.x`) creates those lists of all reference spectra and their parameters (SZA, LOS, RAZ, albedo, latitude, and altitude), that are defined in Table 1.4.1. For each line-of-sight and each latitude, a separate list has to be written. As input for the program, one line-of-sight index (`1e, 2e, 3e, 2n, 1w, 2w, 3w`) and one latitude index (`hila, mila, lola`) are required. The meaning of the indices:

| Index | Line-of-sight [°] |
|---|---|
| `1e` | -34.5 |
| `2e` | -23.0 |
| `3e` | -11.5 |
| `2n` | 0.0 |
| `1w` | 11.5 |
| `2w` | 23.0 |
| `3w` | 34.5 |

| Index | Latitude |
|---|---|
| `hila` | High latitudes |
| `mila` | Mid latitudes |
| `lola` | Low latitudes |

An example output file `ref_spec_list.txt.hila.3w`:

```
* File:  ref_spec_list.txt
* Last modification:  05.05.2003
*
* Purpose:
* - lists all reference spectra to be generated in current directory
* - user input file for make_ref_spec_script.f90
*
* Notes:
* Lines starting with * contain only comments
* Lines starting with + contain reference spectra that already exist
* Lines starting with !  contain reference spectra to be generated
*
************************************************************
* RAZ HGT ALB TOZ
* e 1 00 03
************************************************************
!  201503w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  202003w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  202503w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  203003w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  203503w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  204003w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
!  204503w0300e1 ALB=0.0 PRE=1.0 TEM=0.0
```

Lines starting with `*` contain only comments, lines starting with `+` contain reference spectra, that already exist (this can be defined in the program `write_refspecliststxt.f`), and lines starting with `!` contain reference spectra to be generated (also defined in the program). The string in the first column defines all atmospheric parameters, excluding the latitude, that are needed for the reference spectra. The string is constructed as follows:

`20xxxyyttaarh`, whereas:

`20` → Is fixed, mustn't be changed
`xxx` → Defines the solar zenith angle in tenth degree, e.g. `150`=15°, `905`=90.5°
`yy` → Defines the line-of-sight (`1e, ..., 3w`, see explanation above)
`tt` → Total ozone index (`01` = 125 DU, `02` = 175 DU,..., `10` = 575 DU)
`aa` → Albedo index (`00` = 0.02, `02` = 0.2, `04` = 0.4, ..., `08` = 0.8, and `10` = 0.98)
`r` → Relative azimuth angle (`i` = minimum, `e` = mean, and `a` = maximum)
`h` → Altitude index (`1` = 0 km, `2` = 2 km, ..., `7` = 12 km)

The second column (`ALB=0.0`) defines the albedo again. The third column (`PRE=1.0`) defines the altitude independent scaling factor of the pressure profile. In our case, it is always 1.0. The fourth column (`TEM=0.0`) defines the altitude independent scalar shift [K] of the temperature profile, here always 0.0 K.

The entire line is used as input for the SCIATRAN radiative transfer code.

After having created all lists for each latitude and line-of-sight ($3 \times 7 = 21$ lists alltogether), they have to be put in the beloning directories. That means, `ref_spec_list.txt.hila.w3` has to be copied in the directory `/HIGH_LAT/W3/ref_spec_list.txt` (without the extension `hila.w3`), and so on.

### 4.2.4 Compute reference spectra

The actual computation of the reference spectra is done with the shell script

`make_ref_spec.sh`,

which is created by the program `make_ref_spec_script.f` (executable `make_ref_spec_script.exe`). The shell script then calls SCIATRAN with the correct input line, and the spectra will be created. This has to be done in each of the 21 above mentioned subdirectories.

### 4.2.5 Line-of-sight average and Chebyshev polynomials

If the computation of all reference spectra is completed, they have to be averaged, and the Chebyshev polynomials have to be computed. The programs to do this are listed in the following table for all different types of scan modes. The programs are stored and executed in the directories `/LOW_LAT/`, `/MID_LAT/`, and `/HIGH_LAT`.

| **Pixel Type** | **LOS average** | **Programs** |
|---|---|---|
| **Normal pixel** | | |
| East | E1, E2, E3 | `meanspec_ew_hila.f` and `chebyshev_ew_hila.f` |
| Nadir | E3, N2, W1 | `meanspec_na_hila.f` and `chebyshev_na_hila.f` |
| West | W1, W2, W3 | see east |
| Backscan | W3, W2, W1, N2, E3, E2, E1 | `chebyshev_ba_hila.f` |
| Fullscan (6 sec) | see backscan | see backscan |
| **Small swath width** | | |
| East | -9.45°, -6.3°, -3.15° | `smallscan_ew_hila.f` |
| Nadir | -3.15°, 0.0°, +3.15° | `smallscan_na_hila.f` |
| West | +3.15°, +6.3°, +9.45° | see east |
| Backscan | +9.45°, +6.3°, +3.15°, 0.0°, -3.15°, -6.3°, -9.45° | smallscan_ba_hila.f |
| Fullscan (6 sec) | see backscan | see backscan |
| **Static scan** | | |
| Nadir | N2 | `staticscan_hila.f` |
| **NoCoadd** | | |
| East | -17.25°, -14.375°, -11.5° | `nocoadd_hila.f` |
| Nadir | +5.75°, +8.625°, +11.5° | see east |
| West | +28.65°, +31.625°, +34.5° | see east |
| Backscan | -17.25°, -25.875°, -34.5° | see east |
| **Test scan** | | |
| East | -4.8°, -3.2°, -1.6° | `testscan_hila.f` |
| Nadir | -1.6°, 0.0°, +1.6° | see east |
| West | +1.6°, +3.2°, +4.8° | see east |
| Backscan | +4.8°, +0.0°, -4.8° | see east |
| Fullscan (6 sec) | see backscan | see east |

The last step after the computation of all reference spectra is to create lists of all spectra which contain only the information on all input parameters, e.g.

- name of reference spectrum,
- viewing geometry,
- height,
- albedo,
- surface pressure and temperature,
- ozone, nitrogen dioxide, and bromoxide columns.

Note that the solar zenith angle is set to 1 in all cases, as the reference spectra contain the polynomial coefficients, obtained from a fit through all 34 solar zenith angles, for which the reference spectra have been

computed. The spectrum for a certain solar zenith angle has to be evaluated using the polynomial coefficients. This is done automatically in the `kvant` fitting program.

The program to create such lists is called `update_refspec_list.f`. Before the execution, the list `ref_spec_list.txt` has to be copied in `old_list.txt` (name is fixed). The program then creates a list called `new_list.ref`, which has to be renamed in `ref_spec_list.ref`. `ref_spec_list.ref` is the list used as input for `kvant`. Find below an example file for `ref_spec_list.ref`:

```
*

filename sza los azi grd alb pre tem o3 no2 bro
N
1260
'rs_20szamn0100e1.ref' 1 0.0 0.0 0.0 0.02 1003.8 247.4 0.3384D+19 0.2914D+16 0.1741D+14
'rs_20szamn0200e1.ref' 1 0.0 0.0 0.0 0.02 1003.8 277.6 0.4734D+19 0.2842D+16 0.1694D+14
'rs_20szamn0300e1.ref' 1 0.0 0.0 0.0 0.02 1003.8 277.6 0.6088D+19 0.2784D+16 0.1647D+14
'rs_20szamn0400e1.ref' 1 0.0 0.0 0.0 0.02 1003.8 277.6 0.7440D+19 0.2739D+16 0.1603D+14
'rs_20szamn0500e1.ref' 1 0.0 0.0 0.0 0.02 1003.8 277.6 0.8792D+19 0.2739D+16 0.1603D+14
⋮
```

# Chapter 5

# Ring database

For WFDOAS it is possible to select bewteen two Ring data bases. The so-called old version is a set of 32 Ring spectra (`gtring01.vac, ..., gtring32.vac`), which vary only with the solar zenith angle. All other atmospheric parameters, such as ozone, albedo, and altitude are fixed in this case.

The spectra can be found in the directory

`/wfdoas/Version1/kvant_auxinput/`

The new Ring version contains the full set of Ring spectra, which have been computed with the same settings as the reference data base. The only difference is, that the viewing geometry is limited to nadir due to computational reasons. It has been verified that the variation with LOS is negligible and its small variation can be accounted for by the fitted Ring amplitude.

The Ring spectra can be found in the directories parallel to the reference spectra for each latitude belt:

```
/wfdoas/HIGH_LAT/RING/
/wfdoas/MID_LAT/RING/
/wfdoas/LOW_LAT/RING/
```

The naming of the Ring spectra (`ri_*.ref`) is similar to the naming of the reference spectra (`ref_*.ref`), see subsection 4.2.3.

# Chapter 6

# The kvant program

## 6.1 Compile and run the program

The source code `kvant.f90` can be found in the directory

`/wfdoas/Version1/program/f90/programs/.`

If changes in the source code are performed, compilation is done in the directory

`/wfdoas/Verison1/program/f90/make/`

with `> gmake clean` and `> gmake program=kvant`. The executable `kvant` can be found in `/wfdoas/Verison1/program/f90/bin/`.

The Makefile contains all options for SUN, LINUX, and AIX compilations.

The shell script

`/wfdoas/sh/kvant.sh`

starts the execution of the kvant program from any directory. Call:

`/wfdoas/sh/kvant.sh` *radp_orbit_pixel0_pixel1 outname* `or|nr V1 HDF|ASC SOL|NOSOL`

| | |
|---|---|
| *radp_orbit_pixel0_pixel1* | → The radiance file, must be in the current directory |
| *outname* | → Tag for outputfile(s) |
| `or \| nr` | → Select between old and new Ring version |
| `V1` | → Version (`V1` only at the moment) |
| `HDF \| ASC` | → Select input and output format, HDF or ascii |
| `SOL \| NOSOL` | → `SOL`: solar spectrum from database<br>`NOSOL`: solar spectrum from lv1 file |

Please note, the combination *HDF* and *SOL* is not allowed, as the external solar database, which is stored in the directory

`/wfdoas/solar/`,

is in ascii format only. This database contains the daily mean solar spectra extracted and averaged from the sunpackages contained in the level 1 data. Usually the averaging was done with those 40 spectra that have the highest intensity in the ozone spectral window during the passive and daily tracking of the sun. This solar database circumvents the problems associated with the faulty solar update contained in GOME data in 2002 as provided by the GDP.

The various `kvant` executables for the different platforms are contained in

`/wfdoas/Version1/execute`,

e.g. `kvant.lx` for linux and `kvant.x` for solaris.

## 6.2 The configuration file `kvant.cfg`

The configuration file `kvant.cfg` is the required input for `kvant`. It is generated automatically by the `kvant.sh` script. All settings controlling the program execution are made in this file. It has to be placed in the same directory from which the shell script `kvant.sh` is called.

All lines defining configuration parameters are copied from the configuration file into the main output file header(s). This allows you to repeat a fit using the same settings.

Normally comment lines in `kvant.cfg` are not copied to the main output file. If you want a comment to be copied, precede it with two asterisks instead of one.

Syntax: Text in `typewriter style` has to be written verbatim. *Slanted roman text* denotes a symbolic name for which a value has to be inserted. Square brackets [] enclose optional items. A vertical bar | separates two or more items in a list, from which exactly one has to be selected.

### 6.2.1 Detailed keyword description

The following keywords are available :

`ID, BACKGROUND, CURRENT, TRACE, WFM, WINDOW, DEGPOLY, RINGDB, FRAUNHOFER DO, MODE, EXTOUT, MAINOUT, VERBOSE, VERBOSE2`

With some of these keyword, sub-keywords are used:

`PATH, EXTENSION, FILE, SHSQ_LIMITS, FORMAT, BASEPATH, WF, FILELIST, ITERATE, MEMORY, LIST, REFSPECS`

#### 6.2.1.1 Background spectrum

- `BACKGROUND PATH` *background-path*
  *background-path* is the path to the file(s) containing background spectra.
- `BACKGROUND EXTENSION` *background-extension*
  *background-extension* is the extension of the file(s) containing background spectra. `mea` or `h5` are allowed.

- `BACKGROUND FILE` *background-file*
  The background spectrum will be read from file *background-file*
- `BACKGROUND FORMAT` {`ASC` | `HDF`}
  The format of the background spectrum.

#### 6.2.1.2 Current spectrum

- `CURRENT PATH` *current-path*
  *current-path* is the path to the file(s) containing radiance spectra.
- `CURRENT EXTENSION` *current-extension*
  *current-extension* is the extension of the file(s) containing radiance spectra. `mea` or `h5` are allowed.
- `CURRENT FILE` *current-file*
  The radiance spectrum will be read from file *current-file*
- `BACKGROUND FORMAT` {`ASC` | `HDF`}
  The format of the current spectra.
- `CURRENT SHSQ_LIMITS` *min-sh max-sh [min-sq max-sq]*
  Set the shift and squeeze limits (in nm) for the current spectrum. Shift and squeeze limits are zero by default (no shift and squeeze).

#### 6.2.1.3 DOAS reference spectra

- `TRACE PATH` *trace-path*
  *trace-path* is the path to the file(s) containing the DOAS trace gas reference spectra. *trace-path* is added to relative names only, not to absolute names.
- `TRACE` *id trace-filename [[column-number] degpoly [min-sh max-sh [min-sq max-sq]]]*
  This line contains the definitions for exactly one reference spectrum, e.g. a trace gas absorption cross section, a ring spectrum or an undersampling spectrum.
  *id* is a string of up to 8 characters, is a unique identifier for the reference.
  *trace-filename* is the name of the file containing the reference spectrum in x-y-ASCII format. *trace-path* will be prepended to *trace-filename*.
  *column-number* is the column in *trace-filename*, from which the reference spectrum is to be read. Default is the second column. The wavelength is always read from column 1.
  *degpoly* is the degree of the polynomial, which is subracted from the reference spectrum to make it differential. This happens before the fit. The number of polynomial coeffcients is *degpoly* + 1. By default, *degpoly* = -1, i.e. no individual polynomials are subtracted. This is recommended as it is both redundant and time comsuming.
  *min-sh* and *max-sh* are th shift limits for the reference given in nm. They specify the range, within which the nonlinear fit is allowed to vary the shift parameter for this reference.
  *min-sq* and *max-sq* are the squeeze limits for the reference given in nm. They specify the range within which the nonlinear fit is allowed to vary the squeeze parameter.

#### 6.2.1.4 Weighting function reference spectra

- `WFM BASEPATH` *wfm-path*
  *wfm-path* is the path to the file(s) containing the reference spectra.
- `WFM EXTENSION` *wfm-extension*
  *wfm-extension* is the extension of the file(s) containing the weighting function reference spectra.

- `WFM FILELIST` *wfm-filelist*
  *wfm-filelist* is the list with all information about the weighting function reference spectra, which are available.

- `WFM SHSQ_LIMITS` *min-sh max-sh [min-sq max-sq]*

- `WFM ITERATE` *number-of-iterations*
  *number-of-iterations* is the maximum number of iterations that will be performed.

- `WFM WF` *id priority-parameter* `SUBTRACT`
  *id* is a string of up to 8 characters, which is a unique identifier for the reference.
  *priority-parameter* defines the priority of the parameter with regard to the search for the nearest neighbor reference spectrum. In this specified `kvant` version for ozone retrieval only, is is necessary that the *priority-parameter* for ozone is `1` and that for temperature is tt 0.
  `SUBTRACT`

Note: All those parameters, which are fitted using the weighting functions (ozone and temperature), have to be specified twice, once with the `TRACE` keyword and also with the `WFM WF` keyword ! Those parameters with a slant column fit only (minor absorbers, Ring and undersampling), have to be specified only with the `TRACE` keyword.

#### 6.2.1.5 Ring reference spectra

- `RINGDB MEMORY`
  This keyword is used only for the old Ring version (Parameter *or* is selected for the `kvant.sh` script.

- `RINGDB LIST` *ringlist.txt*
  This keyword is also used only for the old Ring version. *ringlist.txt* is a list of 32 Ring spectra, which vary only with SZA. The molecular filling-in due to ozone is neglected in this case.

- `RINGDB REFSPECS` This keyword is used in case of the new Ring version (parameter *nr* is selected when calling the `kvant.sh` script. Now, the whole Ring data base depending on solar zenith angle, ozone column, latitude, albedo, and altitude is used for the fitting.

#### 6.2.1.6 Preparation of spectra and fit

- `MODE` {`LINEAR` | `SINGLE` | `INDIVIDUAL` | `COUPLED` *min-sh max-sh [min-sq max-sq]* }
  Controls the fit mode, i.e. whether and how the nonlinear parameters shift and squeeze are fitted. the default mode is `LINEAR`. The recommended mod is `SINGLE`. Note that the execution time increases with the number of nonlinear parameters.
  `MODE LINEAR` selects the linear fit mode. Shift and squeeze values are not fitted. Instead they are kept fixed at the mean values of their limits, *(min-sh + max-sh)/2*, and *(min-sq + max-sq)/2*, respectively. This refers both to the current spectrum (limits given with the `CURRENT SHSQ_LIMITS`) and to each reference ( limits given with the `TRACE` keyword.
  `MODE SINGLE` selects a restricted nonlinear fit mode. The current (earth radiance) spectrum is shifted and squeezed within the limits given with the `CURRENT SHSQ_LIMITS` keyword. Shifts and squeezes of the reference spectra are kept fixed at their mean values as described for the linear mode.
  `MODE COUPLED` *min-sh max-sh [min-sq max-sq]* selects a restricted nonlinear fit mode. A common shift and a common squeeze value are fitted for all references, i.e. they are shifted and squeezed together. The given limits are those for the common shift and squeeze values. Their default value is zero. Any shift and squeeze limits for the references given with the `TRACE` keyword are ignored. Note that shift and squeeze for the current spectrum are still determined separately: they are not coupled to those of the references, and their limits have to be specified with the `CURRENT SHSQ_LIMITS` keyword. This mode is not recommended.

`MODE INDIVIDUAL` selects the general nonlinear fit mode. Shift and Squeeze parameters for each reference and for the current spectrum are fitted independently. Shift and squeeze limits for the references are given with the `TRACE` keyword and shift and squeeze limits for the current spectrum are given with the `CURRENT SHSQ_LIMITS` keyword. This mode has to be used with great care as many artifacts may arise.

- `WINDOW` *start-wavelength end-wavelength*
  *start-wavelength* and *end-wavelength* are the approximate margins of the fit window in nm. The fit window must be specified. The actual window depends on the wavelength grid of the background spectrum. It is determined as the largest subset of the grid which lies completely within the specified window. Thus, the actual fit window is always slightly smaller than the specified window. It will be written to screen and output files.

- `DEGPOLY` *overall-polynomial*
  *overall-polynomial* is the degree of the 'overall' polynomial, which is fitted together with the references inthe linear fit. It must not be smaller than the highest 'individual' polynomial degree *degpoly*, given in the *TRACE* keyword. Its default value is 2. the number of polynomial coeffcients is *overall-polynomial* + 1.

- `FRAUNHOFER DO`
  The background (GOME solar) spectrum is nonlinearly fitted to a high resolution solar atlas derived from Fourier transform spectrometer measurements carried out with the McMath Solar Telescope, Kitt Peak Observatory, Arizona (Kurucz *et al.*, 1984). This so-called Fraunhofer fitting is done before the DOAS fit is performed.

#### 6.2.1.7 File and screen output

- `ID` *identifier*
  *identifier* is a string identifying the set of parameters given in the current file.

- `MAINOUT` {`ASC`|`HDF`}
  Select ASCII (`ASC`) or `HDF` output format for the main putput file.

- `MAINOUT PATH` *mainout-path*
  *mainout-path* is the directory into which the main output files will be written.

- `EXTOUT` {`ASC`|`HDF`}
  Select ASCII (`ASC`) ot `HDF` output format for the extended output file.

- `EXTOUT PATH` *extout-path*
  *extout-path* is the directory into which the extended output files will be written.

- `VERBOSE` {`T`|`F`}
  If `T` is selected, screen output is activated, and if `F` is selected, it is omitted.

- `VERBOSE2` {`T`|`F`}
  If `T` is selected, screen output is activated, and if `F` is selected, it is omitted.

## 6.3 Example Configuration file

Calling the shell script

```
/wfdoas/sh/kvant.sh radp_70915171 test nr V1 ASC NOSOL
```

produces the following configuration file

```
** Configuration file for kvant.f90
ID test

*.mea:

BACKGROUND PATH .
BACKGROUND FILE solp_70915171
BACKGROUND EXTENSION mea
BACKGROUND FORMAT ASC

output generated:
<current file>.<ID> Fit results
<current file>.<ID>X Fit results + Residuals

CURRENT PATH .
CURRENT FILE radp_70915171
CURRENT EXTENSION mea
CURRENT FORMAT ASC

CURRENT SHSQ_LIMITS -0.2 0.2 -0.2 0.2

WFM BASEPATH /mnt/raider/wfdoas/Version1
WFM EXTENSION ref
WFM FILELIST ref_spec_list.ref

WFM SHSQ_LIMITS -0.2 0.2 -0.2 0.2

WFM WF O3_ 1 SUBTRACT
WFM WF TEM 0

WFM ITERATE 10

TRACE PATH .
TRACE TEM /mnt/raider/wfdoas/Version1/kvant_auxinput/dummy.filename 5 -1 -0.2 0.2 -0.2 0.2
TRACE O3_ /mnt/raider/wfdoas/Version1/kvant_auxinput/dummy.filename 4 -1 -0.2 0.2 -0.2 0.2
TRACE NO2 /mnt/raider/wfdoas/Version1/kvant_auxinput/n_no2_241.vac 2 -1 -0.2 0.2 -0.2 0.2
TRACE BRO /mnt/raider/wfdoas/Version1/kvant_auxinput/brow298_gpp.dat 2 -1 -0.2 0.2 -0.2 0.2
TRACE RING /mnt/raider/wfdoas/Version1/kvant_auxinput/gtring03.vac 2 -1 -0.2 0.2 -0.2 0.2
TRACE USAM /mnt/raider/wfdoas/Version1/kvant_auxinput/undersampling_o3.dat 2 -1 -0.2 0.2 -0.2
0.2

*** RING A
RINGDB MEMORY
RINGDB LIST /wfdoas/Version1/kvant_auxinput/ringlist.txt

*** RING B
RINGDB REFSPECS

FRAUNHOFER DO

MAINOUT PATH .
MAINOUT ASC

EXTOUT PATH .
```

```
EXTOUT ASC

MODE SINGLE
MODE LINEAR
MODE INDIVIDUAL
MODE COUPLED -0.2 0.2 -0.2 0.2

WINDOW 326.6 335.0

DEGPOLY 3

VERBOSE f
VERBOSE2 f
```

## 6.4 Structure of the main program `kvant`

1. Initialize the configuration variables (Subroutine `InitConfig()`)

2. Read configuration file `kvant.cfg` (Subroutine `ReadConfig()`)

3. Read DOAS reference spectra for $NO_2$, BrO, and the undersampling

4. Read background (solar) spectrum and do the Fraunhofer fit if `FRAUNHOFER DO` keyword is set.

5. Read current (radiance) spectrum and get initial values for ozone, surface temperature, bromoxide, and nitrogen dioxide, as well as the auxiliary information of geolocation, viewing geometry (scan mode), surface pressure, effective altitude and effective albedo.

6. Read list of reference spectra (Subroutine `ReadWfMRefSpecFilelist()`) (separate lists for each latitude and scan mode)

7. Get the nearest neighbor reference and Ring spectra (Subroutine `GetMeanSpectraFromList()`). Perform the linear interpolation between reference spectra for albedo, altitude, relative azimuth angle, and, if required, for latitudes. The latitude $\phi$ of the pixel center defines from which latitude band (high, mid, or low) the ozone profiles will be taken. If $|\phi| > 65^\circ$ high latitude profiles are selected, if $55^\circ > |\phi| > 35^\circ$, mid latitude profiles are taken, and if $|\phi| < 25^\circ$, profiles come from low latitudes. In four ten degree wide transition regions ($\pm 55^\circ$ to $\pm 65^\circ$ and $\pm 25^\circ$ to $\pm 35^\circ$) a linear interpolation between the reference spectra from high and mid latitudes, and from mid and low latitudes, respectively, is performed. In contrast to the reference spectra, no interpolation is done for the Ring spectra.

8. Fitting procedure

   (a) If another reference spectrum can be found, which is closer than the first one, the procedure is repeated with step (7).

   (b) If the fit is finished and the optimum reference spectrum has been found, the ghost vertical column is added, and the output files are written. The next ground pixel (new radiance spectrum) will be processed (step(5)).

## 6.5 The `kvant` output files

`kvant` produces two output files, the so-called main output file and an extended output file. The first contains the whole pixel information and the fit results in terms of vertical columns. Besides the pixel and column information, the extended output file contains also the spectral information for all fit parameters, the optical depth, and the fit residual.

### 6.5.1 Main output file

The main output file of `kvant` contains several header lines, which give an explanation of the different columns in the file. The actual number of header lines and columns in the output file depend on the number of fit parameters defined in the configuration file `kvant.cfg`. Please note, column 1 contains a running index (always starting with 1) of the ground pixels in the WF-DOAS fit, whereas column 6 contains the actual GOME ground pixel number from the level 1 file. Column 2 is the ID of the closest reference spectrum found.

Then follows the information on the size of the actual fit window, which is always within the range defined in the `kvant.cfg` configuration file (keyword WINDOW) and which depends on the wavelength grid of the solar spectrum.

The following part contains the whole `kvant.cfg` file, beginning with `** Configuration file for kvant.f90` and ending with the last keyword `VERBOSE2`. This allows to repeat the fit using exactly the same settings.

At last, the pixel information and the fit results as described in the header lines are listed for each ground pixel.

```
<asc-xy> DOAS fit results
Created by KVANT_WFM - Version 0.x (last modification 15 Oct 2001)
Column 1 = WFM ground pixel number
Column 2 = WFM refspec ID
Column 3 = Pixel quality info
Column 4 = GOME day
Column 5 = GOME time (after midnight) [msec]
Column 6 = Ground pixel
Column 7 = Subset counter
Column 8 = Solar zenith angle (B)
Column 9 = Line-of-sight angle (B)
Column 10 = Relative azimuth (B)
Column 11 = Latitude N (corner 1)
Column 12 = Latitude N (corner 2)
Column 13 = Latitude N (corner 3)
Column 14 = Latitude N (corner 4)
Column 15 = Latitude N (center)
Column 16 = Longitude E (corner 1)
Column 17 = Longitude E (corner 2)
Column 18 = Longitude E (corner 3)
Column 19 = Longitude E (corner 4)
Column 20 = Longitude E (center)
Column 21 = Effective altitude [km]
Column 22 = Surface altitude [km]
Column 23 = Cloud top height [km]
Column 24 = Cloud fraction
Column 25 = Ghost vertical column [DU]
```

```
Column 26 = Total ozone column [DU]
Column 27 = # Sh&Sq iterations
Column 28 = Residual (p2p)
Column 29 = RMS (total)
Column 30 = Fraunhofer shift parameter
Column 31 = TEM linear fit parameter [K]
Column 32 = TEM linear fit error [%]
Column 33 = TEM mean value [K]
Column 34 = O3_ linear fit parameter [molec/cm^2]
Column 35 = O3_ linear fit error [%]
Column 36 = O3_ mean value [molec/cm^2]
Column 37 = NO2 linear fit parameter []
Column 38 = NO2 linear fit error [%]
Column 39 = NO2 mean value []
Column 40 = BRO linear fit parameter []
Column 41 = BRO linear fit error [%]
Column 42 = BRO mean value []
Column 43 = RING linear fit parameter []
Column 44 = RING linear fit error [%]
Column 45 = RING mean value []
Column 46 = USAM linear fit parameter []
Column 47 = USAM linear fit error [%]
Column 48 = USAM mean value []
Column 49 = Current shift [nm]
Column 50 = Current squeeze [nm]
Actual window 326.65--334.97 nm
Configuration file for kvant.f90
ID Include_GVC
BACKGROUND PATH .
BACKGROUND FILE solp_70915171
BACKGROUND EXTENSION mea
CURRENT PATH .
CURRENT FILE radp_70915171
CURRENT EXTENSION mea
CURRENT SHSQ_LIMITS -0.2 0.2 -0.2 0.2
WFM BASEPATH /mnt/raider/wfdoas/Version1
WFM EXTENSION ref
WFM FILELIST ref_spec_list.ref
WFM SHSQ_LIMITS -0.2 0.2 -0.2 0.2
WFM WF O3_ 1 SUBTRACT
WFM WF TEM 0
WFM ITERATE 10
TRACE PATH .
TRACE TEM /wfdoas/Version1/kvant_auxinput/dummy.filename 5 -1 -0.2 0.2 -0.2 0.2
TRACE O3_ /wfdoas/Version1/kvant_auxinput/dummy.filename 4 -1 -0.2 0.2 -0.2 0.2
TRACE NO2 /wfdoas/Version1/kvant_auxinput/n_no2_241.vac 2 -1 -0.2 0.2 -0.2 0.2
TRACE BRO /wfdoas/Version1/kvant_auxinput/brow298_gpp.dat 2 -1 -0.2 0.2 -0.2 0.2
TRACE RING /wfdoas/Version1/kvant_auxinput/gtring03.vac 2 -1 -0.2 0.2 -0.2 0.2
TRACE USAM /wfdoas/Version1/kvant_auxinput/undersampling_o3.dat 2 -1 -0.2 0.2 -0.2 0.2
RINGDB REFSPECS
FRAUNHOFER DO
MAINOUT PATH .
MAINOUT ASC
EXTOUT PATH .
EXTOUT ASC
```

```
MODE SINGLE
WINDOW 326.6 335.0
DEGPOLY 3
VERBOSE f
VERBOSE2 f
1 '20szamn0406e3' 0 19970916.  61883128.  142 3 8.845000E+01 -5.500000E-0 1 -6.979000E+01 7.646000E+
7.620000E+01 8.407000E+01 8.377000E+01 8.02800 0E+01 7.920000E+00 1.103000E+01 3.543000E+01
3.814000E+01 1.762000E+01 4.5 30000E+00 0.000000E+00 6.400000E+00 7.100000E-01 1.040000E+01
2.885504E+02 5 2.405233E-02 4.019849E-03 1.097625E-03 2.534415E+02 2.091793E+00 2.491 451E+02
7.479465E+18 8.665138E-01 7.119582E+18 5.492931E+16 6.830090E+01 0 .000000E+00 -6.538537E+14
3.345548E+01 0.000000E+00 -1.033758E+00 6.309671E+0 0 0.000000E+00 -5.853518E-01 2.811955E+01
0.000000E+00 2.047341E-03 -2.66895 9E-03
2 '20szamn0506e3' 0 19970916.  61889128.  146 3 8.811000E+01 -5.500000E-0 1 -6.976000E+01 7.656000E+
7.632000E+01 8.431000E+01 8.402000E+01 8.04400 0E+01 6.430000E+00 9.590000E+00 3.290000E+01
3.584000E+01 1.569000E+01 3.7 40000E+00 0.000000E+00 8.320000E+00 4.500000E-01 8.330000E+00
3.011627E+02 5 2.166961E-02 3.739774E-03 1.097625E-03 2.592859E+02 1.779831E+00 2.541 020E+02
7.874272E+18 8.585426E-01 8.524116E+18 6.837827E+16 5.134380E+01 0 .000000E+00 -7.890499E+14
2.577436E+01 0.000000E+00 -1.056146E+00 5.754925E+0 0 0.000000E+00 -5.691195E-01 2.690351E+01
0.000000E+00 2.042396E-03 -2.37722 9E-03
⋮
```

### 6.5.2 Extended output file

The extended output file contains the same information as the main output file, except the header and the `kvant.cfg` content. Additionally it contains the spectral information of the target function (optical depth (entire right hand side of equation 1.4.1)), fitted weighting functions (ozone and temperature), DOAS spectra ($NO_2$, BrO, Ring, and undersampling), and the fit residual, which is the difference between left and right hand side of Eq. 1.4.1.

```
*<asc-xy> DOAS extended fit results
Created by KVANT_WFM - Version 0.x (last modification 15 Oct 2001)
Column 1 = Wavelength [nm]
Column 2 = Measured radiance/irradiance [ster⁻1]
Column 3 = Mean radiance/irradiance [ster⁻1]
Column 4 = Fitted polynomial
Column 5 = Fit residual
Column 6 = TEM reference
Column 7 = O3_ reference
Column 8 = NO2 reference
Column 9 = BRO reference
Column 10 = RING reference
Column 11 = USAM reference
Actual window 326.65--334.97 nm *@ 1 '20szamn0406e3' 0 19970916.  61883128.  142 3 8.845000E+01
-5.500000E-01 -6.979000E+01 7.646000E+01 7.620000E+01 8.407000E+01 8.377000E+01 8.028000E+01
7.920000E+00 1.103000E+01 3.543000E+01 3.814000E+01 1.762000E+01 4.530000E+00 0.000000E+00
6.400000E+00 7.100000E-01 1.040000E+01 2.885504E+02 5 2.405233E-02 4.019849E-03 1.097625E-03
2.534415E+02 2.091793E+00 2.491451E+02 7.479465E+18 8.665138E-01 7.119582E+18 5.492931E+16
6.830090E+01 0.000000E+00 -6.538537E+14 3.345548E+01 0.000000E+00 -1.033758E+00 6.309671E+00
0.000000E+00 -5.853518E-01 2.811955E+01 0.000000E+00 2.047341E-03 -2.668959E-03
326.6483 1.62603E-02 2.28525E-02 1.08833E+00 -2.60424E-03 1.28904E-02 3.69410E-01 1.66543E-02
-1.90962E-03 6.09247E-04 1.67828E-03
326.7627 1.64783E-02 2.28940E-02 1.08862E+00 2.39440E-03 1.25324E-02 3.51399E-01 1.65041E-02
-1.78654E-03 5.11704E-03 -1.21707E-03
```

⋮

# Chapter 7

# Acronyms

| Acronym | Meaning |
|---|---|
| AMF | AirMass Factor |
| CDI | Combined Differential Integral |
| DFD | German Remote Sensing Data Centre |
| DLR | German Aerospace Center |
| DOAS | Differential Optical Absorption Spectroscopy |
| DOD | Differential Optical Depth |
| ERS-2 | Second European Remote Sensing Satellite |
| ESA | European Space Agency |
| FRESCO | Fast retrieval Scheme for Clouds from the Oxygen A-band |
| GDP | GOME Data Processor |
| GOME | Global Ozone Monitoring Experiment |
| GOTOCORD | GOME Total Column Retrieval Development |
| GVC | Ghost Vertical Column |
| ICFA | Initial Cloud Fitting Algorithm |
| ISCCP | International Satellite Cloud Climatology Project |
| IUP | Institute of Environmental Physics |
| LER | Lambertian Equivalent Reflectivity |
| LOS | Line-Of-Sight |
| LUT | Look-Up-Table |
| RRS | Rotational Raman Scattering |
| RTM | Radiative Transfer Model |
| SCD | Slant Column Density |
| SCIAMACHY | SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY |
| SRD | Software Requirements Document |
| SZA | Solar Zenith Angle |
| TOA | Top Of Atmosphere |
| TOMS | Total Ozone Mapping Spectrometer |
| UV | Ultraviolet |
| UTC | Coordinated Universal Time (Greenwich Meridian Time) |
| VCD | Vertical Column Density |
| WF-DOAS | Weighting Function DOAS |
| WMO | World Meteorological Organization |
| WOUDC | World Ozone and Ultraviolet Radiation Data Centre |

# Bibliography


BUCHWITZ, M., ROZANOV, V. V., and BURROWS, J. P. 2000. A near-infrared optimized DOAS method for the fast global retrieval of atmospheric $CH_4$, CO, $CO_2$, $H_2O$, and $N_2O$ total column amounts from SCIAMACHY Envisat-1 nadir radiances. *J. Geophys. Res.*, **105**, 15231–15245.

BURROWS, J. P., DEHN, A., DETERS, B., HIMMELMANN, S., RICHTER, A., VOIGT, S., and ORPHAL, J. 1998. Atmospheric remote-sensing reference data from GOME: Part 1. Temperature-dependent absorption cross sections of $NO_2$ in the 231-794 nm range. *J. Quant. Spectrosc. Rad. Transfer*, **60**, 1025–1031.

BURROWS, J. P., RICHTER, A., DEHN, A., DETERS, B., HIMMELMANN, S., VOIGT, S., and ORPHAL, J. 1999. Atmospheric remote-sensing reference data from GOME: Part 2. Temperature-dependent absorption cross sections of $O_3$ in the 231-794 nm range. *J. Quant. Spectrosc. Rad. Transfer*, **61**, 509–517.

COLDEWEY-EGBERS, M., WEBER, M., LAMSAL, L.N., DE BEEK, R., BUCHWITZ, M., and BURROWS, J. P. 2003 (November). *WF–DOAS algorithm theoretical basis document*. Tech. rept. issue 1.2. Institute of Environmental Physics, University of Bremen. ESRIN Contract 16402/02/I-LG.

COLDEWEY-EGBERS, M., WEBER, M., LAMSAL, L. N., DE BEEK, R., BUCHWITZ, M., and BURROWS, J. P. 2004. A novel total ozone algorithm for backscatter UV using the weighting function DOAS approach. *Atmos. Chem. Phys. Discuss.*, **4**, 4915–4944.

DE BEEK, R., WEBER, M., ROZANOV, V. V., ROZANOV, A., RICHTER, A., and BURROWS, J. P. 2004. Trace gas column retrieval – an error study for GOME-2. *Adv. Space Res.*, **34**, 727–733.

HERMAN, J. R., and CELARIER, E. A. 1997. Earth surface reflectivity climatology at 340-380 nm from TOMS data. *J. Geophys. Res.*, **102**(D23), 28003–28011.

KOELEMEIJER, ¡R. B. A., STAMMES, P., HOVENIER, J. W., and DE HAAN, J. F. 2001. A fast method for retrieval of cloud parameters using oxygen A-band measurements from the Global Ozone Monitoring Experiment. *J. Geophys. Res.*, **106**, 3475–3496.

KURUCZ, R. L., FURENLID, I., BRAULT, J., and TESTERMAN, L. 1984. *Solar flux atlas from 296 nm to 1300 nm*. National Solar Observatory, Sunspot, New Mexico.

ROOZENDAEL, M. VAN, SOEBIJANTA, V., FAYT, C., and LAMBERT, J.-C. 2003. *Investigation of DOAS issues affecting the accuracy of the GDP version 3.0 total ozone product*. unpublished manuscript, see Chapter VI of http://earth.esrin.esa.it/pub/ESA_DOC/GOME/gdp3/gdp3.htm.

ROZANOV, V. V., DIEBEL, D., SPURR, R. J. D., and BURROWS, J. P. 1997. GOMETRAN: A radiative transfer model for the satellite project GOME, The plane-parallel version. *J. Geophys. Res.*, **102**, 16683–16695.

ROZANOV, V. V., KUROSU, T., and BURROWS, J. P. 1998. Retrieval of atmospheric constituents in the UV/visible: A new analytical approach to calculating weighting functions. *J. Quant. Spectrosc. Rad. Transfer*, **60**, 277–299.

SLIJKHUIS, S., VAN BARGEN, A., THOMAS, W., and V.CHANCE, K. 1999. Calculation of Undersampling correction spectra for DOAS spectral fitting. *Pages 563–569 of:* ESA (ed), *Esams'99 - european symposium on atmospheric measurements from space*. ESA, Noordwijk, The Netherlands.

WEBER, M., LAMSAL, L. N., COLDEWEY-EGBERS, M., BRAMSTEDT, K., and BURROWS, J. P. 2004a. Pole-to-pole validation of GOME WFDOAS total ozone with groundbased data. *Atmos. Chem. Phys. Discuss.*, **xxx**, xxx–xxx.

WEBER, M., LAMSAL, L.N., COLDEWEY-EGBERS, M., BRAMSTEDT, K., and VANICEK, K. 2004b (January). *WF–DOAS version 1.0 validation report*. Tech. rept. issue 1.2. Institute of Environmental Physics, University of Bremen. ESRIN Contract 16402/02/I-LG.

WEBER, M., LAMSAL, L.N., and COLDEWEY-EGBERS, M. 2004c (January). *WFDOAS V1.0 delta-validation report*. Tech. rept. issue 1.0. Institute of Environmental Physics, University of Bremen. ESRIN Contract 16402/02/I-LG.

WELLEMEYER, C. G., TAYLOR, S. L., SEFTOR, C. J., MCPETERS, R. D., and BHARTIA, P. K. 1997. A correction for the Total Ozone Mapping Spectrometer profile shape errors at high latitude. *J. Geophys. Res.*, **102**, 9029–9038.