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**GOME Software Databases
for
Level 1 to 2 Processing**

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Document Change Log

Rev.	Date	Section	Description of Change	approved by	Sign
1/A	15.7.93	all	Completely new		
1/B	15.10.93	all	Comments of the review meeting participants and project members are included		
2/A	15.12.00	all	Update of data bases and inclusion of new data bases reflecting the operational version GDP L12 2.7		
3/A	31.07.02	all	Update of data bases and inclusion of new data bases reflecting the operational version GDP L12 3.0		

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1 Introduction

This technical note contains summary descriptions of the climatological and spectroscopic data bases required for the execution of the GOME Level 1 to 2 Data Processing Chain. Data bases have been taken directly from the GOMEware (the scientific software developed for GOME processing) package and from other literature sources.

GOME Level 1 to 2 software data bases are divided into 6 general classes as follows:

Cross–section databases:	Absorption cross–sections for GOME trace gases including Ring;
Surface databases:	Global surface albedo, global vegetation index, global topography, other surface reflectance data;
Profile databases:	Pressure, temperature, trace gas concentration profiles;
Spectroscopic databases:	Slit function, O ₂ optical depths, other reference spectra such as undersampling correction pseudo– cross–sections;
Aerosol data bases:	Particle loading, attenuation properties, phase functions;
Cloud databases:	Cloud top reflectances, particle extinction and scattering properties.

Section 2 outlines the information contained in the summary descriptions – each database is characterised with a brief description followed by notes on units, dimensions and errors (the latter where applicable). Some remarks follow on the purpose and usage of the data, and on the control parameters for data base extraction. The software notes supply the name of the FORTRAN 77 Block Data file in which the data set appears, plus the format and approximate size of the corresponding object file. Every data set contains at least one source reference.

Sections 3 and 4 contain summaries for all those GOME databases which are *essential* for the operational Level 1 to 2 processing chain (the DOAS total column retrieval process). Section 3 is devoted to cross–sections only, with separate entries for each trace gas species (including Ring); section 4 deals with essential data bases from the other five general classes.

In the interests of completeness, summary tables of those databases not directly used in the GDP retrieval algorithm are gathered in the Appendix A. Some of these are additional data bases required for the simulation of GOME Level 1 data; some will be needed for more sophisticated profile retrieval algorithms. Mention is made of the application of these data sets in scientific and testing contexts (for example with the raw data simulator).

Appendix B is a compilation of source references for the special scenarios data set.

Special thanks are due to R. Guzzi (surface data), D. Diebel (special scenarios, cross–section data base review), K. Chance (solar spectra, BrO Ring, theoretical Ring, air–to–vacuum– corrected BrO, BrO FTS, HCHO FTS, BrO undersampling correction), J. Lavagnino (GOMEware programming), T. Kurosu (cloud top reflectances), A. Richter (hand–shifted and air–to–vacuum– corrected O₄, air–to–vacuum– corrected OCIO), M. Vountas (theoretical Ring), A. Türk/M.Eisinger (SO₂ BBM), J. Orphal (O₃ FTS), P. Stammes (document review).

2 Explanation of Data Base Summaries

The following notes are intended as a guide to the data base summaries.

Type of Data base	Surface, Profiles, Cross–sections, Spectroscopic, Aerosols, Clouds
Name of Data Set	Brief name (3 to 5 words).
Description	Concise scientific description of contents (each part is described separately).
Dimensions/Size	Number of data points and dimensions of defining arrays (for example number of wavelengths at which cross sections are specified). [Sub–sections of the data bases may have different dimensions].
Physical Units	Units for the data quantities. These are standardised wherever possible – for example, all trace gas concentration profiles are expressed as number mixing ratios, all cross sections (except O ₄) have units cm ² .mol ⁻¹ . Not all data have physical units (indices, unit less ratios, etc.).
Reference/Source	Journal or document reference given where possible. Private communications are mentioned in full.
Error	An a priori error value can be assigned to most climatological data inputs to retrieval and sensitivity analyses; this is mentioned explicitly in the text. For cross–sections, an examination of the source references has yielded a mixed bag of error specifications; some in percent, some as 2–sigma confidence, while others are absent. (Percent unless otherwise specified).
Functional usage	Indication of application of data base in main Level 1 to 2 software algorithms (e.g. concentration profile input to Air Mass Factor routine, input reference spectra to DOAS fitting algorithm, etc.). Some data sets have several applications.
Selection Control	Indication of controlling parameters for the selection of appropriate extractions from the data bases. In many cases, these are the geolocation parameters (time, viewing geometry, surface locations). Other parameters may be fixed (e.g. trace gas molecule flags). The term "discretion" means operator–controlled input, and as such does not apply to the GOME <i>operational</i> processing chain.
Data Library	Name of the Block data file which contains data base. All files have the extension ".f", except the special scenarios data base (extension ".PAR").
Software Format	Variable type, precision of format, size of Fortran 77 object file. All format specifications are taken from Fortran 77 language definition.
Other remarks	As appropriate.

3 Cross–section Data Bases

3.1 BrO cross–sections

Cross–section data bases are presented in alphabetical order for the trace gas absorbers in the GOME range.

Type of Data Base	Cross–section
Name of Data Set	BrO absorption cross–section
Description	Wavelengths and Absorption Cross–sections for trace gas BrO.
Dimensions/Size	1926 Cross–section values from 312.372 to 388.257 nm, resolution 0.04 nm. Total entries 2 x 1926.
Physical Units	cm ² .mol ⁻¹ .
Errors	0.1 nm on wavelength. 1–sigma error 8%.
Reference Source	[A51]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross–sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of BrO as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F10.5 wavelengths, 1PE13.7 cross–sections. Size of Database 16.983 Kb.
Other Remarks	The original spectrum has been modified due to the air–to–vacuum shift (Edlen 1966) and it has been hand–shifted by 0.17nm towards longer wavelengths (Richter 2000).

3.2 CIO cross-sections

Type of Data Base	Cross-section
Name of Data Set	CIO absorption cross-section
Description	Wavelengths and Absorption Cross-sections for trace gas CIO.
Dimensions/Size	937 Cross-section values from 236.518 to 312.385 nm, resolution 0.081 nm. Total entries 2 x 937.
Physical Units	cm ² .mol ⁻¹ .
Errors	1-sigma 5–10%
Reference Source	[A37]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of CIO as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 7.496 Kb.
Other Remarks	

3.3 HCHO cross-sections

Type of Data Base	Cross-section
Name of Data Set	HCHO absorption cross-section
Description	Wavelengths and Absorption Cross-sections for trace gas HCHO.
Dimensions/Size	5048 Cross-section values from 224.58 to 375.99 nm, resolution 0.004 nm. Total entries 2 x 5048.
Physical Units	cm ² .mol ⁻¹ .
Errors	Not available.
Reference Source	[A26]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of HCHO as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 41.944 Kb.
Other Remarks	

3.4 NO₂ cross-sections

Type of Data Base	Cross-section
Name of Data Set	NO₂ absorption cross-section (part 1)
Description	Wavelengths and Absorption Cross-sections for trace gas NO ₂ .
Dimensions/Size	20387 Cross-section values from 200.1 to 709.75 nm, resolution 0.025 nm. Total entries 2 x 20387.
Physical Units	cm ² .mol ⁻¹ .
Errors	0.01 nm quoted for wavelength. 3% (500–600 nm), 13% (200–250 nm).
Reference Source	[A37]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of NO ₂ as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 163.096 Kb.
Other Remarks	Some doubt over wavelength registration of these results.

Type of Data Base	Cross–section
Name of Data Set	NO₂ absorption cross–section (part 2)
Description	Wavelengths and Absorption Cross–sections for trace gas NO ₂ at 7 temperatures
Dimensions/Size	1748 Cross–section values from 313.1 to 567.73 nm, resolution 0.14 nm. Total entries 2 x 1748 x 7 = 24472
Physical Units	cm ² .mol ⁻¹ .
Errors	Wavelength accuracy around 0.1nm. Cross–section errors between 1% and 15%, depending on temperature regime (see paper for details).
Reference Source	[A20]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross–sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of NO ₂ as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format E10.5 wavelengths, 1PE10.5 cross–sections. Size of Database 220.634 Kb.
Other Remarks	The data base includes data from 4 grating positions and therefore there are 3 discontinuities in the wavelength axis. These occur at 380.905 nm, 440.93 nm and 501.03 nm.

3.5 NO₃ cross-sections

Type of Data Base	Cross-section
Name of Data Set	NO₃ absorption cross-section
Description	Wavelengths and Absorption Cross-sections for trace gas NO ₃ .
Dimensions/Size	341 Cross-section values: (a) from 400.0 to 599.0 nm at resolution 1.0 nm (200 data points) and (b) from 600.0 to 670.0 nm at resolution 0.5 nm. Total entries 2 x 341.
Physical Units	cm ² .mol ⁻¹ .
Errors	13%
Reference Source	[A37], [A29], [A53]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of NO ₃ as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 2.728 Kb.
Other Remarks	

3.6 O₂ cross-sections

Type of Data Base	Cross-section
Name of Data Set	O₂ absorption cross-section
Description	Wavelengths and Absorption Cross-sections for O ₂ .
Dimensions/Size	1456 Cross-section values from 650.0 to 795.5 nm at resolution 0.1 nm. Total entries 2 x 1456.
Physical Units	cm ² .mol ⁻¹ .
Errors	TBD
Reference Source	[A8]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of O ₂ as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 11.648 Kb.
Other Remarks	The use of cross-sections for the O ₂ absorption in the A and B bands (760 and 687 nm) is a poor substitute for the more accurate line by line treatment. This data set is not used in the cloud pre-processing algorithm. The AMF for O ₂ is a useful indicator for the radiation path length.

3.7 O₄ cross-sections

Type of Data Base	Cross-section
Name of Data Set	O2–O2 absorption cross-section
Description	Wavelengths and Absorption Cross-sections for O2–O2 collision complex
Dimensions/Size	(a) 3770 Cross-section values from 300.087 to 677.087 nm at resolution 0.1 nm; (b) 902 values from 1000.0 to 1136.0 nm at resolution 0.1/0.2 nm. Total entries 2 x (3770+902) = 9344.
Physical Units	cm ⁵ .molecule ⁻² . Scaled by factor 10 ⁺⁴⁰ .
Errors	10% (2-sigma confidence).
Reference Source	[A17]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of O2–O2 as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F10.5 (a), F8.3 (b) wavelengths, 1PE11.5 (a), 1PE13.7 (b) cross-sections. Size of Database 38.934 Kb.
Other Remarks	The first segment (a) has been corrected for the air-to-vacuum shift and it has been hand-shifted by Richter ([A30]) by about 1nm towards longer wavelengths. Additionally, steps have been removed by interpolation.

3.8 O₃ cross-sections

Type of Data Base	Cross-section
Name of Data Set	O₃ absorption cross-sections (part 1)
Description	Wavelengths and Absorption Cross-sections for O ₃ .
Dimensions/Size	(a) 5122 points from 184.9277 to 253.7595 nm at resolution 0.134 nm (<i>short-wave</i>); (b) 2408 points from 253.7749 to 365.3635 nm at resolution 0.0357 rising to 0.06 nm (<i>Hartley–Huggins</i>); (c) 4373 points from 407.8 nm to 845.0 nm at resolution 0.1 nm (<i>Chappuis</i>).
Physical Units	cm ² .mol ⁻¹ .
Errors	(a) not known; (b) 0.025 nm wavelength, 1% cross-section; (c) none available.
Reference Source	[A55], [A2], [A56], [A22]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms. Vertical total column of O ₃ is the key output of GDP Level 1 to 2 Processing.
Control Selection	Presence of O ₃ controlled by logical molecule flags, with a separate flag set for O ₃ as a retrieval species. For wavelengths in the Hartley–Huggins range, suitable temperatures are required to perform the "Bass–Paur" fit to the true O ₃ cross-section.
Data Library	GSPECLIB.f
Software Format	ASCII Real Numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of data set 95.224 Kb.
Other Remarks	For other Hartley–Huggins coefficients, see next page.

Type of Data Base	Cross–section
Name of Data Set	O₃ absorption cross–sections (part 2)
Description	First and second order fitting coefficients for the Hartley–Huggins Absorption Cross–sections for O ₃ .
Dimensions/Size	2 coefficients at 2408 points from 253.7749 to 365.3635 nm at resolution 0.0357 rising 0.06 nm. Total 2 x 2408 points.
Physical Units	K ⁻¹ cm ² mol ⁻¹ (first coefficient); K ⁻² cm ² mol ⁻¹ (second coefficient).
Errors	Complete cross sections (including temperature correction 1%
Reference Source	[A2], [A27]
Functional Usage	Coefficients used to correct for the true O ₃ cross–section in the Hartley–Huggins wavelengths.
Control Selection	Invoked only for wavelengths in the Hartley–Huggins range (253–365 nm, but mainly significant above 335 nm). Otherwise control as for O ₃ cross–sections (see previous page).
Data Library	GSPECLIB.f
Software Format	ASCII Real Numbers. Format F8.4 wavelengths, 1PE13.7 cross–sections. Size of data set 19.264 Kb.
Other Remarks	Total size of data base = 114.488 Kb.

3.9 OCIO cross-sections

Type of Data Base	Cross-section
Name of Data Set	OCIO absorption cross-sections
Description	Wavelengths and Absorption Cross-sections for trace gas OCIO.
Dimensions/Size	2923 Cross-section values from 242.59 to 472.80 nm at resolution 0.072 nm. Total entries 2 x 3210.
Physical Units	cm ² .mol ⁻¹ .
Errors	7% (2-sigma confidence)
Reference Source	[A51]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of OCIO as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 27.256 Kb.
Other Remarks	Low-temperature spectrum chosen (trace gas only present in special circumstances, at these temperatures). Data has been air-to-vacuum corrected by Richter ([A30]).

3.10 SO₂ cross-sections

Type of Data Base	Cross-section
Name of Data Set	SO₂ absorption cross-section
Description	Wavelengths and Absorption Cross-sections for trace gas SO ₂ .
Dimensions/Size	5625 Cross-section values from 227.34 to 339.82 nm, resolution 0.02 nm. Total entries 2 x 5625.
Physical Units	cm ² .mol ⁻¹ .
Errors	less than 2%.
Reference Source	[A21]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of SO ₂ as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 45.0 Kb.
Other Remarks	

3.11 H₂O cross-sections

Type of Data Base	Cross-section
Name of Data Set	H₂O Continuum
Description	Wavelengths and Absorption Coefficients for trace gas H ₂ O (self- and foreign-broadened contributions to continuum spectrum).
Dimensions/Size	1602 points for wavelengths and contributions from self-broadening term at 296K, self-broadening term at 260K and Foreign-broadening term at 296K. Range 500.0 nm to 2506.266 nm at resolution 20 cm ⁻¹ . Total entries 6 x 1602.
Physical Units	cm ³ .mol ⁻¹ . Scaled by 10 ⁻²⁰
Errors	5–25%
Reference Source	LOWTRAN data compilation, [A23].
Functional Usage	Not used in DOAS. Interpolated to GOME wavelengths, coefficients required for calculation of optical depths in AMF and other radiative transfer algorithms.
Control Selection	H ₂ O is not yet selected as a contributing species above 500 nm, as it is necessary to compute the line absorption <i>in addition</i> to the continuum (not yet implemented).
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F8.4 wavelengths, 1PE13.7 cross-sections. Size of Database 38.448 Kb.
Other Remarks	This continuum data is largely empirical.

Type of Data Base	Cross–section
Name of Data Set	H₂O Cross–sections
Description	Wavelengths and Absorption Coefficients for trace gas H ₂ O.
Dimensions/Size	39053 points for wavelengths and cross–sections at 280 K from 409.48 nm to 800.99 nm. Total entries 2 x 39053.
Physical Units	cm ² .mol ⁻¹ .
Errors	5–25%
Reference Source	HITRAN 1992 data compilation carried out by K. Chance, October 26, 1993, [A35]
Functional Usage	Reference spectrum in DOAS fitting algorithm below 500nm; also cross–sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of H ₂ O as a contributing species is controlled by a logical flag.
Data Library	GSPECLIB.f
Software Format	ASCII real numbers. Format F6.2 wavelengths, 1PE10.4 cross–sections. Size of Database 314.007 Kb.
Other Remarks	The spectrum has been calculated from HITRAN 1992 line–by–line data at 0.9 atm (= 911.7 hPa) and 280 K using a Gaussian instrument width. The spectrum has been splined out to 0.01nm resolution using Numerical Recipes ([A28]) routines SPLINE and SPLINT. There are 10 segments (gaps in wavelength) but data is logically ordered in one big segment.

3.12 Ring spectra

Type of Data Base	Cross–section
Name of Data Set	Theoretical Ring (SAO)
Description	Wavelengths and pseudo cross–sections for Rotational Raman Scattering (Ring).
Dimensions/Size	7801 points for cross–sections from 237.00 nm to 310.99 nm, 9501 points for cross–sections from 311.00 nm to 393.99 nm, 21701 points for cross–sections from 394.00 nm to 577.99 nm, and 21701 points for cross–sections from 578.00 nm to 795.00 nm. Total entries 60704. In addition, 4 wavelengths at the beginning of each spectral segment and the (constant) spectral resolution are given.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F6.2 wavelengths, 1PE10.4 cross–sections. Size of Database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is an absolute spectrum that must be transformed internally into a differential spectrum.
Type of Data Base	Cross–section

Name of Data Set	Theoretical Ring (SAO) – BrO window
Description	Wavelengths and pseudo cross–sections for Rotational Raman Scattering (Ring) for BrO fitting with molecular contributions from O ₂ and N ₂ .
Dimensions/Size	2501 entries for cross–sections and wavelengths from 340.00 nm to 365.00 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for BrO fitting as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.10 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is an absolute spectrum that must be transformed internally into a differential spectrum.

Name of Data Set	Theoretical Ring (SAO) – ozone window (first EV, GOME)
Description	Wavelengths and pseudo cross–sections (first Eigenvector) for Rotational Raman Scattering (Ring) for ozone fitting, based on a GOME sun spectrum (Orbit 17296).
Dimensions/Size	177 entries for cross–sections and wavelengths from 319.986 nm to 340.072 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is a differential spectrum.

Name of Data Set	Theoretical Ring (SAO) – ozone window (second EV, GOME)
Description	Wavelengths and pseudo cross-sections (second Eigenvector, molecular contributions from O ₂ and N ₂) for Rotational Raman Scattering (Ring) for ozone fitting, based on a GOME sun spectrum (Orbit 17296).
Dimensions/Size	144 entries for cross-sections and wavelengths from 319.986 nm to 336.337 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo-species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.05 cross-sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is a differential spectrum.

Name of Data Set	Theoretical Ring (SAO) – ozone window (first EV, Fraunhofer)
Description	Wavelengths and pseudo cross–sections (first Eigenvector) for Rotational Raman Scattering (Ring) for ozone fitting, based on a high resolution Fraunhofer spectrum (Kurucz).
Dimensions/Size	2001 entries for cross–sections and wavelengths from 320.00 nm to 340.00 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is a differential spectrum.

Name of Data Set	Theoretical Ring (SAO) – ozone window (second EV, Fraunhofer)
Description	Wavelengths and pseudo cross–sections (second Eigenvector, molecular contributions from O ₂ and N ₂) for Rotational Raman Scattering (Ring) for ozone fitting, based on a high resolution Fraunhofer spectrum (Kurucz).
Dimensions/Size	2001 entries for cross–sections and wavelengths from 320.00 nm to 340.00 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is a differential spectrum.

Name of Data Set	Theoretical Ring (SAO–IASB) – ozone window (first EV, GOME)
Description	Wavelengths and pseudo cross–sections (first Eigenvector) for Rotational Raman Scattering (Ring) for ozone fitting, based on a GOME solar spectrum using a Gaussian slit function with FWHM = 0.162.
Dimensions/Size	175 entries for cross–sections and wavelengths from 320.98 nm to 339.96 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10], [A32]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format 1PE12.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is a differential spectrum, given as raman/solar.

Name of Data Set	Theoretical Ring (SAO–IASB) – Channel 2 (first EV, GOME)
Description	Wavelengths and pseudo cross–sections (first Eigenvector) for Rotational Raman Scattering (Ring) for ozone fitting, based on a GOME solar spectrum using a Gaussian slit function with FWHM = 0.162.
Dimensions/Size	828 entries for cross–sections and wavelengths from 312.676 nm to 405.119 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10], [A32]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format 1PE12.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is an absolute spectrum, given as raman/solar (normalized).

Name of Data Set	Theoretical Ring (SAO–IASB) – Channel 3 (first EV, GOME)
Description	Wavelengths and pseudo cross–sections (first Eigenvector) for Rotational Raman Scattering (Ring) for ozone fitting, based on a GOME solar spectrum using a Gaussian slit function with FWHM = 0.162.
Dimensions/Size	955 entries for cross–sections and wavelengths from 407.026 nm to 608.591 nm, respectively.
Physical Units	–
Errors	N/A
Reference Source	[A10], [A32]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of Theoretical Ring spectrum for ozone fitting window as a contributing pseudo–species is controlled by a logical flag.
Data Library	GSAORING.f
Software Format	ASCII real numbers. Format 1PE12.5 wavelengths, 1PE12.05 cross–sections. Size of entire database 314.300 Kb.
Other Remarks	The theoretical Ring spectrum given here is an absolute spectrum, given as raman/solar (normalized).

Name of Data Set	IFE – Theoretical Ring
Description	Wavelengths and pseudo cross–sections (two eigenvectors) for Rotational Raman Scattering (Ring).
Dimensions/Size	2447 points for first eigenvector from 237.523 nm to 607.918 nm, 2447 points for cross–sections from 237.523 nm to 607.918 nm. Total entries 4 x 2447 for two eigenvectors.
Physical Units	–
Errors	N/A
Reference Source	[A50]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the eigenvectors as contributing pseudo–species is controlled by a logical flag.
Data Library	GIFERING.f
Software Format	ASCII real numbers. Format F6.2 wavelengths, 1PE12.5 cross–sections. Size of entire Database 40.028 Kb (including second eigenvector).
Other Remarks	The two eigenvectors given here are already in differential form and must not be filtered in the DOAS kernel.

Type of Data Base	Cross–section
Name of Data Set	GOME BBM SO₂
Description	Wavelengths and cross–sections for SO ₂ measured by the GOME Bread–Board model (BBM).
Dimensions/Size	1024 points for wavelengths and cross–sections from 286.62 – 410.236 nm at 298 K. Total entries 2 x 1024 = 2048 entries.
Physical Units	cm ² .mol ⁻¹ .
Errors	N/A
Reference Source	[A48]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the SO ₂ BBM spectrum as a contributing species is controlled by a logical flag.
Data Library	GBBMDATALIB.f
Software Format	ASCII real numbers. Format F7.3 wavelengths, 1PE9.3 cross–sections. Size of Database 9.029 Kb.
Other Remarks	<p>The wavelength grid is the vacuum wavelength grid.</p> <p>Gas Handling: Flow system allows the adjustment of calibrated flows of trace gas and dilution gas (syn. air) Cell: Multiple reflection quartz cell with an optical path length of 985 cm Spectrometer: GOME BBM (Channel #2) Detection: GOME BBM (Reticon Diode array) Light Source: 30 W Deuterium lamp Integration Time: 30 & 36 sec</p>

Type of Data Base	Cross–section
Name of Data Set	FTS O3
Description	Wavelengths and cross–sections for O ₃ measured by FTS.
Dimensions/Size	12168 points for wavelengths and cross–sections from 236.404 – 415.800 nm at 203 K, 12168 points for wavelengths and cross–sections from 236.404 – 415.800 nm at 223 K, 12168 points for wavelengths and cross–sections from 236.404 – 415.800 nm at 246 K, 12168 points for wavelengths and cross–sections from 236.404 – 415.800 nm at 280 K, and 12168 points for wavelengths and cross–sections from 236.404–415.800 nm nm at 293 K. Total entries are 2 x 60840 = 121680.
Physical Units	cm ² .mol ⁻¹ .
Errors	see reference.
Reference Source	[A49]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the O ₃ FTS spectrum as a contributing species is controlled by a logical flag.
Data Library	GFTS_O3LIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE10.3 cross–sections. Size of data base 487.652 Kb.
Other Remarks	<p>The wavelength grids are the vacuum wavelength grids.</p> <p>Remarks from J. Orphal: The resolution of the FTS data was 20.0 cm⁻¹ (original FTS data recorded at 5 cm⁻¹ un–apodized resolution). The original FTS data were convoluted with a Gaussian function of 20.0 cm⁻¹ FWHM. This corresponds to a resolution of about 0.2 nm in the UV region. The convolution was applied in order to reduce noise and to match (approximately) the resolution of the GOME FM data.</p> <p>After convolution, the FTS spectra were corrected for low–frequency baseline errors using the GOME FM spectra at corresponding temperatures. This was achieved by least–squares fitting where the FTS data was corrected with a low–order polynomial baseline and the GOME FM data were shifted/squeezed. This approach was selected because it obviously reduces systematic errors in the available data. The GOME FM data contains wavelength–uncertainties and some sampling problems – the FTS data does not. However, the FTS data contains baseline problems due to lamp drifts – the GOME FM data is much better in this respect. Thus, it is appropriate to correct the FTS data for baseline problems and the GOME FM data for wavelength shifts in a simultaneous fit.</p>

Type of Data Base	Cross–section
Name of Data Set	FTS BrO
Description	Wavelengths and cross–sections for BrO measured by FTS.
Dimensions/Size	6094 points for wavelengths and cross–sections from 286.380 – 383.047 nm at 228 K. Total entries are $2 \times 6094 = 12188$.
Physical Units	$\text{cm}^2 \cdot \text{mol}^{-1}$.
Errors	see reference.
Reference Source	[A54]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the BrO FTS spectrum as a contributing species is controlled by a logical flag.
Data Library	GFTS_BROLIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE14.6 cross–sections. Size of data base 49.592 Kb.
Other Remarks	The wavelength grids are the vacuum wavelength grids. There are data sets with different spectral resolution available. Here, the measurements with 10 cm^{-1} (no apodization) have been integrated, following a suggestion from K. Chance.

Type of Data Base	Cross–section
Name of Data Set	FTS HCHO
Description	Wavelengths and fit coefficients (temperature parameterization) for HCHO measured by FTS.
Dimensions/Size	15018 points for wavelengths and cross–section coefficients from 300.305 – 385.786 nm. Total entries are 3 x 15018 = 45054.
Physical Units	cm ² .mol ⁻¹ .
Errors	see reference.
Reference Source	[A9]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the HCHO FTS spectrum as a contributing species is controlled by a logical flag.
Data Library	GFTS_HCHOLIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE11.4 cross–sections. Size of data base 181.060 Kb.
Other Remarks	The wavelength grid is the vacuum wavelength grid. The cross–sections are calculated from the two coefficient data sets using a linear function of temperature ($\sigma = \text{coeff}_1 + \text{coeff}_2 * T$). The selected HCHO temperature is typically 250 K, to reflect the higher tropospheric content of HCHO. It has been realised that there may occur unphysical negative values for the final HCHO cross–sections at certain wavelengths.

3.13 O₃ Flight Model (FM) cross-sections (1996)

Type of Data Base	Cross-section
Name of Data Set	GOME FM96 O₃
Description	Wavelengths and cross-sections for O ₃ measured by the GOME Flight Model (FM) – 1996.
Dimensions/Size	3331 points for wavelengths and cross-sections from 230.984 – 794.256 nm at 202 K, 3330 points for wavelengths and cross-sections from 230.984 – 794.256 nm at 221 K, 3332 points for wavelengths and cross-sections from 230.990 – 794.281 nm at 241 K, 3339 points for wavelengths and cross-sections from 230.864 – 794.281 nm at 273 K, and 3332 points for wavelengths and cross-sections from 231.117 – 793.409 nm at 293 K. In addition, the temperature dependency of ozone cross-sections in the Hartley–Huggins bands has been parameterized by a quadratic function of the temperature and fit coefficients are stored. An equally spaced wavelength grid with a constant resolution of 0.1nm is given from 235.00 – 370.00 nm and three coefficients are given for each spectral point. Total entries are 2 x 16664 = 33328 entries for the cross-sections itself and 4 x 1351 = 5404 entries are given for the coefficient data set.
Physical Units	cm ² .mol ⁻¹ .
Errors	N/A
Reference Source	[A6]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of the O ₃ FM 1996 spectrum as a contributing species is controlled by a logical flag. The usage of the cross-sections itself or the temperature parameterization (and the coefficients data base) is controlled by a logical flag.
Data Library	GFMDATALIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE10.4 cross-sections. Size of entire FM 1996 data base 278.133 Kb.
Other Remarks	The wavelength grids are the vacuum wavelength grids.

3.14 NO₂ Flight Model (FM) cross-sections (1996)

Type of Data Base	Cross-section
Name of Data Set	GOME FM96 NO₂
Description	Wavelengths and cross-sections for NO ₂ measured by the GOME Flight Model (FM) – 1996.
Dimensions/Size	3406 points for wavelengths and cross-sections from 230.989 – 794.246 nm at 221 K, 3406 points for wavelengths and cross-sections from 230.985 – 793.846 nm at 241 K, 3408 points for wavelengths and cross-sections from 230.985 – 794.264 nm at 273 K, and 3406 points for wavelengths and cross-sections from 230.993 – 794.214 nm at 293 K. Total entries are 2 x 13826 = 27256.
Physical Units	cm ² .mol ⁻¹ .
Errors	N/A
Reference Source	[A2]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of the NO ₂ FM 1996 spectrum as a contributing species is controlled by a logical flag.
Data Library	GFMDATALIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE10.4 cross-sections. Size of entire FM 1996 data base 278.133 Kb.
Other Remarks	The wavelength grids are the vacuum wavelength grids. The temperature is selected in the initialisation file. There is no interpolation between the temperature blocks. Instead, the nearest neighbour in temperature is used to select the appropriate spectrum.

3.15 Ring Flight Model (FM) cross-sections (1996)

Type of Data Base	Cross-section
Name of Data Set	GOME FM96 Ring
Description	Wavelengths and pseudo- cross-sections for Rotational Raman Scattering (Ring) measured by the GOME Flight Model (FM) – 1996.
Dimensions/Size	764 points for wavelengths and pseudo- cross-sections from 320.189 – 405.168 nm and 838 points for wavelengths and pseudo-cross-sections from 405.206 – 580.985 nm. Total entries are 2 x 1602 = 3204 covering GOME channels #2 and #3.
Physical Units	–
Errors	N/A
Reference Source	[A6]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the Ring FM 1996 spectrum as a contributing species is controlled by a logical flag.
Data Library	GFMDATALIB.f
Software Format	ASCII real numbers. Format F7.3 wavelengths, 1PE13.6 cross-sections. Size of entire FM 1996 data base 278.133 Kb.
Other Remarks	<p>The wavelength grids are the vacuum wavelength grids. The Ring spectrum is already a differential spectrum which must be treated in a different way than absolute spectra in the DOAS kernel (no polynomial filtering required).</p> <p>Remarks from A. Richter (IFE): Measurements were carried out on 23 September 1994 (morning set). Lower wavelength limit of GOME FM Ring spectrum (channel 2) was found to be greater than the lower limit of the DOAS–UV fitting window used in GDP. The GOME FM Vacuum spectrum was extended to lower wavelengths in the UV to allow Ring reference spectrum to be fitted in DOAS. The UV values at these lower wavelengths were not included originally because of suspected contamination with O₃ absorption structures. Though these may be present, it was decided to extend the data set rather than 'faking' the data or altering the window definition or trying to work in possible theoretically-calculated Ring cross-sections.</p>

3.16 O₃ Flight Model (FM) cross-sections (1998)

Type of Data Base	Cross-section
Name of Data Set	GOME FM98 O3
Description	Wavelengths and cross-sections for O ₃ measured by the GOME Flight Model (FM) – 1998.
Dimensions/Size	3330 points for wavelengths and cross-sections from 230.984 – 794.047 nm at 202 K, 3329 points for wavelengths and cross-sections from 230.984 – 794.047 nm at 221 K, 3332 points for wavelengths and cross-sections from 230.864 – 794.072 nm at 241 K, 3337 points for wavelengths and cross-sections from 230.864 – 793.863 nm at 273 K, and 3337 points for wavelengths and cross-sections from 230.864 – 794.036 nm at 293 K. In addition, the temperature dependency of ozone cross-sections in the Hartley–Huggins bands has been parameterized by a quadratic function of the temperature and fit coefficients are stored. An equally spaced wavelength grid with a constant resolution of 0.1 nm is given from 235.00 – 370.00 nm and three coefficients are given for each spectral point. Total entries are 2 x 16665 = 33330 entries for the cross-sections itself and 4 x 1351 = 5404 entries are given for the coefficient data set.
Physical Units	cm ² .mol ⁻¹ .
Errors	see reference.
Reference Source	[A8]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of the O ₃ FM 1998 spectrum as a contributing species is controlled by a logical flag. The usage of the cross-sections itself or the temperature parameterization (and the coefficients data base) is controlled by a logical flag.
Data Library	GFM98LIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.5 cross-sections. Size of entire FM 1998 data base 265.206 Kb.
Other Remarks	The wavelength grids are the vacuum wavelength grids.

3.17 NO₂ Flight Model (FM) cross-sections (1998)

Type of Data Base	Cross-section
Name of Data Set	GOME FM98 NO2
Description	Wavelengths and cross-sections for NO ₂ measured by the GOME Flight Model (FM) – 1998.
Dimensions/Size	3406 points for wavelengths and cross-sections from 230.989 – 794.246 nm at 221 K, 3408 points for wavelengths and cross-sections from 230.985 – 794.264 nm at 241 K, 3408 points for wavelengths and cross-sections from 230.985 – 794.264 nm at 273 K, and 3408 points for wavelengths and cross-sections from 230.993 – 794.214 nm at 293 K. Total entries are 2 x 13630 = 27260.
Physical Units	cm ² .mol ⁻¹ .
Errors	see reference.
Reference Source	[A7]
Functional Usage	Reference spectrum in DOAS fitting algorithm; also cross-sections required for calculation of trace gas absorption in the AMF and other radiative transfer algorithms.
Control Selection	Presence of the O ₃ FM 1998 spectrum as a contributing species is controlled by a logical flag.
Data Library	GFM98LIB.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, 1PE12.5 cross-sections. Size of entire FM 1998 data base 265.206 Kb.
Other Remarks	The wavelength grids are the vacuum wavelength grids.

3.18 Operational default

3.18.1 Issue 2/A – GDP 2.7

The following settings for DOAS fitting are used as operational default :

UV window (325–335 nm)	
Molecule	Data base
Ozone	GOME FM 1996
Ring	GOME FM 1996

VIS window (425–450 nm)	
Molecule	Data base
Ozone	GOME FM 1996
Ring	Theoretical Ring spectrum (SAO)
Water vapour	Hitran
Nitrogen dioxide	GOME FM 1998
O ₂ –O ₂ collision complex	Greenblatt et al.
Undersampling correction (see 4.3)	Slijkhuis et al.

The ozone Bass–Paur temperature is derived from the height level where the ozone concentration (in number density units) is maximum. In the UV window, the quadratic parameterization as suggested by Bass and Paur is applied to calculate the ozone cross–sections from pre–calculated and stored fit coefficients. Available undersampling spectra are described in section 4.3 of this document.

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The following settings for DOAS fitting are used as operational default :

UV window (325–335 nm)	
Molecule	Data base
Ozone (241 K)	GOME FM 1998, [A8]
Ozone (241–221 K)	GOME FM 1998, [A8]
Nitrogen dioxide	GOME FM 1998, [A7]
Ring (first component)	[A10]
Undersampling correction	[A43]

VIS window (425–450 nm)	
Molecule	Data base
Ozone (221 K)	GOME FM 1998, [A8]
Nitrogen dioxide	GOME FM 1998, [A7]
Ring (first component)	[A10]
Water vapour	[A35]
O ₂ –O ₂ collision complex	[A17], [A30]
Undersampling correction (see 4.3)	[A43]

An effective ozone cross–section temperature is determined as an intermediate result of the spectral fitting. However, this quantity is not part of the GOME level 2 product.

4 General Climatological Data bases

The remaining data bases essential to the GDP Level 1 to 2 processing are summarised in this chapter, in the following order:

4.1 Surface data bases

4.2 Profile data bases

4.3 Spectroscopic data bases

4.4 Aerosol data bases

4.5 Cloud data bases

4.6 AMF LUT

4.1 Surface data bases

4.1.1 Surface albedo and vegetation index

Type of Data Base	Surface
Name of Data Set	Global Surface Albedo and Vegetation Index.
Description	(a) Lambertian <i>wavelength-independent</i> albedo of the earth surface. (b) Classification of land surface type ("Vegetation" index).
Dimensions/Size	1° x 1° Latitude/Longitude grid; total of 180 x 360 entries. Each entry has an encoded value for information about one surface location: albedo values at 4 times of the year, plus the vegetation index. Albedo indices are converted into the actual albedo values using an index table.
Physical Units	None. Albedo values are fractions (2 decimal places); vegetation indices for 31 different land surface types, from 1 (tropical rain forest) to 31 (ocean).
Errors	<i>a priori</i>
Reference Source	[A24]
Remarks on Usage	(a) Ground albedo climatology in cloud pre-processing algorithm. Optional surface boundary condition in the AMF and other radiative transfer algorithms. (b) Optional used in the processing algorithms. Indirect use (1) to determine the boundary layer aerosol type (according to the LOW-TRAN classification scheme) and (2) in the selection of wavelength-dependent surface albedo (classified according to land surface type).
Control Selection	Surface location (latitude & longitude) of the central position of the GOME ground pixel (geolocation information). Presence of the global albedo model is controlled by a keyword in the initialisation file.
Data Library	GSURFGLBLIB.f
Software Format	ASCII integer numbers (4-byte). Format I8. Size of data set 259.2 Kb.
Other Remarks	

4.1.2 Surface reflectance

Type of Data Base	Surface
Name of Data Set	Surface Reflectance
Description	Lambertian <i>wavelength-dependent</i> albedo for various <i>land</i> surface types.
Dimensions/Size	Albedos for 5 different land surfaces (water, soil, vegetation, sand, snow), specified at 86 wavelengths across GOME range (resolution <i>ca.</i> 15 nm). Total 6 x 86 points.
Physical Units	None. Albedo values are fractions (3 decimal places).
Errors	see reference below
Reference Source	[A3], Data compiled by R. Guzzi, IMGA–CNR, 1994
Remarks on Usage	Surface boundary condition in radiative transfer algorithms (including AMF). Alternative to global surface albedo data (which are <i>wavelength-independent</i>).
Control Selection	Discretion for general use of data set. Surface location of ground pixel to select vegetation index, which is then reduced to one of the above 5 categories. Alternative selection of land surface type by discretion. Interpolation over wavelength is required.
Data Library	GSURFLIB.f
Software Format	ASCII real numbers. Formats: wavelength F6.2, albedo F5.3. Size of data set 2.064 Kb.
Other Remarks	The index table for conversion from the global vegetation index (31 values) to one of the above 5 land surfaces is also found in Data Library GSURFLIB.f

4.1.3 Global topography

Type of Data Base	Surface
Name of Data Set	Global Topography
Description	Height of earth land surfaces (above mean sea level).
Dimensions/Size	1° x 1° Latitude/Longitude grid., 180 x 360 entries.
Physical Units	Meters. Heights given to nearest meter. Sea level is zero.
Errors	Not Known
Reference Source	NOAA ETOPO5 data set. Original data resolved at 5 minutes of arc, degraded to present resolution by T. Ruppert, DLR.
Remarks on Usage	(1) Lowest height in cloud pre-processing algorithm. (2) Lower limit of altitude grid in Air Mass Factor calculation and other radiative transfer algorithms.
Control Selection	Surface location (latitude & longitude) of the central position of the GOME ground pixel (geolocation information).
Data Library	GTOPOLIB.f
Software Format	ASCII Integer numbers, Format I4 (largest value 5800). Size of data set 259.2 Kb.
Other Remarks	

4.1.4 Glitter Reflectance

Type of Data Base	Surface
Name of Data Set	Glitter Reflectance
Description	Albedo for glitter–reflected <i>sea</i> surface.
Dimensions/Size	Albedo for sea surface, 5 different wind speeds, 30 different incident zenith angles, 25 wavelengths across GOME range (resolution 25 nm). Total 5 x 30 x 25 points. Data set also includes reference wavelengths, wind speeds and angles (61 points).
Physical Units	Wind speeds in $\text{m}\cdot\text{s}^{-1}$. Angles in degrees. Wavelengths in nm. Albedo values are fractions (4 decimal places).
Errors	<i>A priori</i>
Reference Source	[A19]
Remarks on Usage	Ocean surface boundary condition in radiative transfer algorithms (see below).
Control Selection	Geolocation – surface location of ground pixel selects sea surface, viewing geometry the incident angle. Wind speed by discretion – default 10 m/sec. Interpolation over wavelength is required.
Data Library	GSURFLIB.f
Software Format	ASCII real numbers. Formats: wavelength F6.2, angles F4.1, winds F4.1, albedo F6.4. Size of data set ~ 15.4 Kb.
Other Remarks	Note that the glitter albedo in this data set (despite the lack of knowledge of wind speed) is recommended for use in the models over the single albedo of 0.05 for all angles and wavelengths assumed from the global data base of surface albedo. DISORT has been used to generate the data set.

4.2 Profile data bases

4.2.1 Altitude grids

Type of Data Base	Profile
Name of Data Set	Reference Altitude Grids
Description	Reference altitude grids for use in radiative transfer algorithms (including AMF module).
Dimensions/Size	12 grids with varying number of levels. The default AMF reference grid has 71 levels from 0 to 70 km (composite of MPI grid below 60km and USA grid in upper layers above 61km, resolution 1km). Total number of points <i>ca.</i> 565.
Physical Units	Kilometres.
Errors	<i>A priori</i>
Reference Source	(MPI) [A4], (USA) [A1]
Remarks on Usage	Grids on which input climatological profiles must be interpolated. Layering structure will be altered to accommodate (i) non-zero topography, or (ii) cloud top as the lowest layer, or (iii) presence of other cloud layers.
Control Selection	AMF reference grid is an automatic default.
Data Library	GLAYERSLIB.f
Software Format	ASCII real numbers. Format F5.1 (1 decimal place). Size of data set <i>ca.</i> 3.04 Kb.
Other Remarks	Other grids in this database are used to define climatological profile inputs to radiative transfer simulations (GOMETRAN, DISORT, etc.).

4.2.2 MPI data set

Type of Data Base	Profile
Name of Data Set	MPI Pressure, Temperature, Trace Gas Concentration Profiles
Description	Pressure, temperature and trace gas concentration profiles on a fixed pressure surface altitude grid.
Dimensions/Size	34 pressure levels. 18 latitude zones (every 10°) (a) Pressure/Temperature, 12 monthly values. 2 x 34 x 216 points. (b) Trace gases, 8 species and 4 seasonal values. 8 x 34 x 72 points. (c) Reference height grid, 72 points.
Physical Units	Temperatures in degrees K, pressures in hPa, height in km, concentration profiles as volume number mixing ratios.
Errors	<i>A priori</i>
Reference Source	[A4]
Remarks on Usage	(a) Pressure and Temperature to calculate air density and humidity. Temperature profile values optionally used to set up Ozone cross-sections for wavelengths in the Hartley–Huggins bands. (b) Climatological trace gas profiles are converted to density units (molecules/cm ³) before input to the Air Mass Factor and other radiative transfer algorithms.
Control Selection	Logical variable DO_MPI is the overall flag for the use of the MPI profiles. If this is set, then ground pixel geolocation information (surface location and time) will determine the correct latitude zone and time of year.
Data Library	GPROLIB.f
Software Format	ASCII real numbers. Formats: 4 DP (pressure), 5 DP (temperature), 5 DP (concentrations; Format 1PE13.7). Size of entire profile data set 180.673 Kb.
Other Remarks	MPI profiles only extend to <i>ca.</i> 61 km. For altitude grids up to 100 km, it is necessary to merge MPI profiles (smoothly!) with suitable profiles from the set of USA atmospheres for levels above 61 km.

4.2.3 USA data set

Type of Data Base	Profile
Name of Data Set	USA Pressure, Temperature, Trace Gas Concentration Profiles
Description	Pressure, temperature and trace gas concentration profiles on a fixed pressure surface altitude grid.
Dimensions/Size	46 pressure levels. 6 latitude zones (every 30°, starting with – 75 deg), 8 species (a) Pressure/Temperature/Species, 6 atmospheres (tropical, midlatitude–summer, midlatitude–winter, arctic–summer, arctic–winter, US–Standard), 3 x 6 x 8 x 46 points (b) Reference height grid, 46 points
Physical Units	Temperatures in degrees K, pressures in hPa, height in km, concentration profiles as number mixing ratios.
Errors	see reference below
Reference Source	[A1]
Remarks on Usage	(a) Pressure and temperature to calculate air density and humidity. Temperature profile values optionally used to set up Ozone cross-sections for wavelengths in the Hartley–Huggins bands. (b) Climatological trace gas profiles are converted to density units (molecules/cm ³) before input to the Air Mass Factor and other radiative transfer algorithms.
Control Selection	Automatic – these atmospheres are always required for the higher levels, and for those gases not represented in the MPI data set (e.g. SO ₂ not in the MPI data set). Ground pixel geolocation information (surface location and time) will set the correct atmosphere, except for the <i>USA Standard atmosphere</i> , which has its own logical control flag. Logical variable DO_USA is the overall flag for the use of the USA profiles. If this is set, then ground pixel geolocation information (surface location and time) will determine the correct latitude zone and time of year.
Data Library	GPROLIB.f
Software Format	ASCII real numbers. Formats: 1PE13.7 for pressure, F9.4 for temperature, F9.4 for height grid, 1PE13.7 for concentrations.
Other Remarks	Profiles from this data used to fill the upper atmosphere above 61km or 0.3hPa, respectively, if the MPI data set is used and the input atmospheric height is higher than the maximum height given in that data base.

4.2.4 KNMI data set

Name of Data Set	KNMI Pressure, Ozone Profiles, Standard Deviation
Type of Data Base	Profile
Description	Single reference pressure profile, ozone concentration profiles and its standard deviation on the fixed pressure grid.
Dimensions/Size	19 altitude levels from 0.3 hPa to 1000 hPa 100 km. 17 latitude belts (each 10 deg, starting at –80 deg), 12 monthly mean profiles, same resolution for the standard deviation.
Physical Units	Pressure in hPa, reference latitudes in deg., ozone concentrations as number mixing ratios, standard deviation dimensionless
Errors	see reference below.
Reference Source	[A14]
Remarks on Usage	(a) Pressure profile used to convert from pressure levels to height levels. (b) Climatological ozone profiles are converted to density units (molecules/cm ³) before input to the Air Mass Factor and other radiative transfer algorithms.
Control Selection	Logical variable DO_KNMI is the overall flag for the use of the KNMI profiles. If this is set, then ground pixel geolocation information (surface location and time) will determine the correct latitude zone and time of year.
Data Library	GPROLIB.f
Software Format	ASCII real numbers. Formats: F7.1 for pressure, F5.1 for reference latitudes, I3 used for reference days (of the year), 1PE11.4 for concentrations. Size of entire profile data set 180.673 Kb.
Other Remarks	The KNMI climatology includes ozone hole conditions during Antarctic spring. Upper atmosphere entries filled with appropriate USA ozone concentrations.

4.2.5 TOMS data set

Name of Data Set	TOMS Pressure, Temperature & Ozone Profiles
Type of Data Base	Profile
Description	Pressure, temperature and ozone concentration profiles on the fixed pressure grid.
Dimensions/Size	11 midpoint Umkehr layer altitudes (infinity=0 to 2.8), 11 heights at boundaries of Umkehr layers (48.4112 to 0.), 11 midpoint Umkehr layer pressures (infinity=0 to 716.0), 11 pressures at boundaries of Umkehr layers (0.99 to 1013.0), 6 total columns for tropical scenarios (225 – 475 DU, $\Delta=50$ DU), 10 total columns for midlatitude and arctic scenarios, respectively (125 – 575 DU, $\Delta=50$ DU), 10 profiles with cumulative ozone columns at 12 layers for midlatitude and arctic scenarios, respectively, 6 profiles with cumulative ozone columns at 12 layers for tropical scenarios, 10 profiles with temperatures at 12 layers for midlatitude and arctic scenarios, respectively, 6 profiles with temperatures at 12 layers for tropical scenarios, 11x11 Umkehr layer covariance matrix.
Physical Units	Altitudes in km, pressure in hPa, reference latitudes in deg., ozone concentration in DU.
Errors	see reference below.
Reference Source	[A25]
Remarks on Usage	(a) Pressure profile used to convert from pressure levels to height levels. (b) Climatological ozone profiles are converted to density units (molecules/cm ³) before input to the Air Mass Factor and other radiative transfer algorithms. (c) Only radiative transfer models GOMETRAN ([A36]) and LI-DORT ([A44]) have an interface to the TOMS profiles. The data base is not used in the operational context. (d) The training data set for the neural network has been generated using TOMS ozone and temperature/pressure profiles.
Control Selection	Logical variable DO_TOMS is the overall flag for the use of the TOMS profiles. If this is set, then ground pixel geolocation information (surface location and time) will determine the correct latitude zone and time of year.
Data Library	GTOMSV7LIB.f
Software Format	ASCII real numbers. Formats: F8.2 for pressure, F5.1 for reference altitudes, F6.1 for total columns and cumulative columns, F6.1 used for temperatures, F6.1 for covariance matrix. Size of entire profile data set 4.26 Kb.
Other Remarks	The TOMS climatology contains profiles for ozone hole conditions. Upper atmosphere levels and lowest level down to the ground are filled with appropriate USA ozone concentrations.

4.3 Spectroscopic data bases

4.3.1 Slit function coefficients

Type of Data Base	Spectroscopic
Name of Data Set	Slit Function coefficients
Description	Slit function coefficients for GOME Channels for various slit function types.
Dimensions/Size	8 spectral channel limits (4 channels), 8 pixel limits for active pixels in each channel (4 channels), 3 slit function types (simple–hyperbolic, compound–hyperbolic, exponential). Ca. 80 points
Physical Units	No units.
Errors	see reference.
Reference Source	(a) simple–hyperbolic: [R1], page 37, Version 4: In flight slit functions as determined on May 23rd 1995 (b) compound–hyperbolic: [R1], page 38, Version 4: In flight slit functions as determined on May 23rd 1995 (c) exponential: [R1], page 21
Remarks on Usage	To calculate the slit function that is used to convolve each reference spectrum (high–resolution FTS spectra, other literature sources) that has not been measured by the GOME FM or the GOME BBM.
Control Selection	Application of convolution controlled by a logical flag
Data Library	GSLITLIB.f
Software Format	ASCII real numbers. Formats: F7.4 for slit function coefficients, F5.1 for channel limits, I4 for active pixels. Size of data set 1.5 Kb.
Other Remarks	The simple–hyperbolic slit function type is used operationally.

4.3.2 O₂ A band templates

Type of Data Base	Spectroscopic
Name of Data Set	O₂ A band template data base
Description	Slant path factors for O ₂ absorption in the A band, for various penetration depths (layers), wavelength grid for template transmittances, transmittance templates for 16 atmospheric layers.
Dimensions/Size	17 atmospheric levels, pressure and temperature profile on that grid, 11001 spectral points and 11001 x 16 transmittance values, 16 reference sun zenith angles, 16 x 16 path factors.
Physical Units	Transmittances and path factors are unitless. Height grid in km, pressure grid in hPa, temperature grid in K, spectral grid in nm, reference angles in deg.
Errors	N/A
Reference Source	(a) Slant path factors calculated by an enhanced version of GOME-TRAN (see [5]), including a quasi-spherical treatment of the incoming radiation (b) [A31]
Remarks on Usage	Cloud pre-processing algorithm; optical depths to be convolved with the slit function to simulate transmissions in the O ₂ A band.
Control Selection	Automatic.
Data Library	GTEMPLATESLIB.fb
Software Format	ASCII real numbers. Size of data base 750.279 kB.
Other Remarks	O ₂ transmittances derived from line-by-line calculations using the spectral data base mentioned in (b) in the range of the O ₂ A-band.

4.3.3 Ozone undersampling

Type of Data Base	Spectroscopic
Name of Data Set	O₃ undersampling
Description	Wavelengths and pseudo–cross–sections to correct for interpolation errors in the standard ozone fitting window.
Dimensions/Size	365 points for wavelengths and pseudo–cross–sections from 324.03 – 365.048 nm. Total entries are 2 x 365 = 730.
Physical Units	–
Errors	N/A
Reference Source	[A43]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the O ₃ undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Spectrum calculated as differential spectrum from Kurucz high–resolution sun spectrum and varying FWHM of the slit function (FWHM=0.18/0.16 nm before/after 330.0 nm)

4.3.4 Nitrogen dioxide undersampling

Type of Data Base	Spectroscopic
Name of Data Set	NO₂ undersampling
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard NO ₂ fitting window.
Dimensions/Size	165 points for wavelengths and pseudo– cross–sections from 420.150 – 454.857 nm. Total entries are 2 x 165 = 330.
Physical Units	–
Errors	N/A
Reference Source	[A34]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the NO ₂ undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Spectrum calculated as differential spectrum from Kurucz high–resolution sun spectrum and a slitwidth of FWHM = 0.3 nm.

4.3.5 Bromine monoxide undersampling

Type of Data Base	Spectroscopic
Name of Data Set	BrO undersampling (DLR)
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard BrO fitting window.
Dimensions/Size	163 points for wavelengths and pseudo– cross–sections from 341.196 – 359.354 nm. Total entries are 2 x 163 = 326.
Physical Units	–
Errors	N/A
Reference Source	[A43]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the BrO undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Spectrum calculated as differential spectrum from Kurucz high–resolution sun spectrum and a slitwidth of FWHM = 0.15 nm.

Type of Data Base	Spectroscopic
Name of Data Set	BrO undersampling (SAO–1)
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard BrO fitting window.
Dimensions/Size	189 points for wavelengths and pseudo– cross–sections from 341.984 – 363.024 nm. Total entries are $2 \times 189 = 376$.
Physical Units	–
Errors	N/A
Reference Source	[A11]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the BrO undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Bi–modal differential correction spectrum (first part).

Type of Data Base	Spectroscopic
Name of Data Set	BrO undersampling (SAO–2)
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard BrO fitting window.
Dimensions/Size	189 points for wavelengths and pseudo– cross–sections from 341.984 – 363.024 nm. Total entries are $2 \times 189 = 376$.
Physical Units	–
Errors	N/A
Reference Source	[A11]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the BrO undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Bi–modal differential correction spectrum (second part). Only used together with first part (see page before).

4.3.6 Formaldehyde undersampling

Type of Data Base	Spectroscopic
Name of Data Set	HCHO undersampling
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard HCHO fitting window.
Dimensions/Size	365 points for wavelengths and pseudo– cross–sections from 324.030 – 365.048 nm. Total entries are $2 \times 365 = 730$.
Physical Units	–
Errors	N/A
Reference Source	[A43]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the HCHO undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Spectrum calculated as differential spectrum from Kurucz high–resolution sun spectrum and a slitwidth of $\text{FWHM} = 0.16 \text{ nm}$.

4.3.7 Sulphur dioxide undersampling

Type of Data Base	Spectroscopic
Name of Data Set	SO2 undersampling
Description	Wavelengths and pseudo– cross–sections to correct for interpolation errors in the standard So2 fitting window.
Dimensions/Size	131 points for wavelengths and pseudo– cross–sections from 315.027 – 329.973 nm. Total entries are 2 x 131 = 262.
Physical Units	–
Errors	N/A
Reference Source	[A43]
Functional Usage	Reference spectrum in DOAS fitting algorithm.
Control Selection	Presence of the SO2 undersampling correction is controlled by a logical flag.
Data Library	GSAMPLE.f
Software Format	ASCII real numbers. Format F9.5 wavelengths, F13.10 pseudo–cross–sections. Size of entire data base 14.219 Kb.
Other Remarks	Spectrum calculated as differential spectrum from Kurucz high–resolution sun spectrum and a varying slitwidth of FWHM = 0.26 nm for $\lambda < 320.8$ nm, FWHM = 0.22 nm for $\lambda < 325.2$ nm, and FWHM = 0.18 nm for $\lambda > 325.2$ nm.

4.4 Aerosol data bases

4.4.1 Aerosol loading

Type of Data Base	Aerosol
Name of Data Set	Aerosol Profile Loadings
Description	Aerosol extinction profiles at 550 nm on fixed altitude grids for the 4 LOWTRAN aerosol regimes (boundary layer 0–2 km, tropospheric regime 2–10 km, stratospheric regime 10–30 km, mesospheric regime 30–100 km).
Dimensions/Size	(a) boundary layer 3 height levels, 5 default visibilities; (b) troposphere 8 height levels, 2 seasonal values, 2 default visibilities; (c) stratosphere 16 height levels, 2 seasonal values, 4 types of loading based on volcanic ash density; (d) mesosphere 7 height levels, 2 loading types defaulted to underlying stratospheric loading type. Total points 230.
Physical Units	km ⁻¹ (extinction units). Height and visibility in km.
Errors	<i>A priori</i>
Reference Source	[A40], [A41]
Remarks on Usage	Climatological aerosol profile input to the Air Mass Factor algorithm (extinction only) and other radiative transfer models (extinction and absorption). Profiles at other wavelengths are found by multiplying these 550nm profiles by suitable normalisation factors (see next page).
Control Selection	(a) Boundary layer selected from visibility (default depends on land surface type); (b) Tropospheric values selected from seasonal value (geolocation information and visibility (default = 50 km); (c) Stratospheric values selected from season and from direct choice of particle loading (default in GDP is "background stratospheric"); (d) mesospheric defaulted to stratospheric type.
Data Library	GAERLIB.f
Software Format	ASCII real numbers. Format; height and visibility 1 DP, all profiles 1PE8.2. Size of entire data set 14.557 Kb.
Other Remarks	The use of 550 nm extinction profiles and suitable normalisation factors cannot be changed (data taken from LOWTRAN).

4.4.2 Aerosol spectral properties

Type of Data Base	Aerosol
Name of Data Set	Aerosol Spectral coefficients
Description	Aerosol extinction and absorption normalisation coefficients. Aerosol asymmetry parameters.
Dimensions/Size	All 3 quantities specified at 6 wavelengths covering GOME range. (a) boundary layer: 4 relative humidities, 4 aerosol attenuation regimes ("rural", "maritime", "urban", "tropospheric"). 288 points. (b) troposphere: 4 relative humidities. 72 points. (c) stratosphere: 3 volcanic aerosol attenuation regimes (GDP default to "background stratospheric"). 54 points. (d) mesosphere: 1 default value. 18 points.
Physical Units	Reference wavelengths in nm. Humidity as percentage. All aerosol spectral coefficients are unitless (the extinction and absorption values are normalisation factors).
Errors	<i>A priori</i>
Reference Source	[A40], [A41]
Remarks on Usage	Extinction profiles interpolated to given wavelength is input to the AMF algorithm. Climatological aerosol profiles input to the Air Mass Factor and other radiative transfer algorithms. Asymmetry factors used to compose aerosol phase functions (but not for AMF algorithm).
Control Selection	Boundary layer type selected from land surface type (vegetation index). Stratospheric type from direct input (default in GDP is "background stratospheric"). Other regimes defaulted. Relative humidity profile computed from climatological pressure, temperature and H ₂ O concentration profiles.
Data Library	GAERLIB.f
Software Format	ASCII real numbers. Formats: wavelength F5.1, humidity F4.2, aerosol quantities F7.5. Size of entire data set 14.557 Kb.
Other Remarks	(see previous page)

4.4.3 Aerosol Mie scattering properties

Type of Data Base	Aerosol
Name of Data Set	Aerosol Mie Phase Functions
Description	Aerosol phase functions calculated from a Mie particle scattering model (LOWTRAN data). Aerosols classified as for profiles (see previous two pages).
Dimensions/Size	All values specified at 34 scattering angles from 0° to 180°. Aerosol regime options as for Spectral coefficients (see previous page). 5 reference wavelengths cover the GOME spectral range. Total of 70 phase functions available (2380 data points).
Physical Units	Reference wavelengths in nm. Humidity as percentage. Scattering angles in degrees. Phase function values in (Steradian) ⁻¹ ; all phase functions are normalised to 1.
Errors	<i>A priori</i>
Reference Source	[A40], [A41]
Remarks on Usage	Aerosol scattering property in the AMF algorithm (input phase function profile made up of appropriate Mie phase functions for each of the 4 aerosol regimes).
Control Selection	Selection controlled by a truth table, which indexes correct phase functions according to wavelength and humidity (130 entries).
Data Library	GAERLIB.f
Software Format	ASCII real numbers. Formats: wavelength F5.1, humidity F4.2, phase functions 5 DP. Truth table entries are integers, Format I2. Size of entire data set 14.557 Kb.

4.5 Cloud data bases

4.5.1 Cloud–top reflectances

Type of Data Base	Cloud
Name of Data Set	Tropospheric Clouds: Cloud–top Reflectances
Description	Bi–directional reflectance coefficients for a selection of incident zenith angles, reflected zenith angles and relative azimuths. Specified for a number of cloud scattering asymmetry parameters.
Dimensions/Size	Reflectances given for 8 asymmetry values from 0.830 to 0.865, 7 incident and reflected zenith angles from 0° to 90°, 12 azimuth angles from 0° to 180°. The table for asymmetry values classified according to 8 different low cloud types and 25 wavelengths across the GOME range (200–800 nm at resolution 25nm). Total $(8 \times 7 \times 7 \times 12) + (25 \times 8) = 4904$ points.
Physical Units	unitless ratios
Errors	<i>A priori</i>
Reference Source	[A45], results validated against [A12].
Remarks on Usage	(a) To calculate average climatologic albedo (input to the cloud pre–processing algorithm). (b) Direct input (along with reference angles) to the AMF algorithm; reflection boundary condition in the presence of low clouds.
Control Selection	(a) Automatic. Cloud type is pre–defined at the start of the cloud processing algorithm, and an average cloud top albedo (over the asymmetry values) is taken. Geolocation information provides the correct viewing angles. (b) AMF calculation is done with or without clouds–as–reflecting–boundaries. In the latter case, geolocation information again supplies the viewing geometry, and wavelengths are those corresponding to the mid–points of the DOAS fitting windows.
Data Library	GRHOLIB.f
Software Format	ASCII real numbers. Formats: F5.1 wavelengths, F5.4 asymmetry values, F6.2 angles, F7.4 reflectance coefficients. Size of data base ~19.6 Kb.
Other Remarks	Stored values are reflectances times the cosine of the incident angle. The 8 cloud types and its physical properties are taken from [A47].

4.5.2 ISCCP cloud–top pressure

Type of Data Base	Cloud
Name of Data Set	ISCCP data base
Description	Monthly mean values of cloud–top pressure as function of latitude/longitude.
Dimensions/Size	Reference grids of latitude and longitude with 72 and 144 entries, respectively (spatial resolution of 2.5 x 2.5 degrees), cloud–top pressure values per month, latitude, longitude. Total entries = 72 x 144 x 12 = 20736.
Physical Units	cloud–top pressure in hPa, latitude/longitude reference values in deg.
Errors	see references
Reference Source	(a) [A38], (b) [A33]
Remarks on Usage	Used for the computation of the cloud–top height which is an essential input for the AMF module (AMF to cloud–top).
Control Selection	Automatic.
Data Library	GISCCPLIB.f
Software Format	ASCII real numbers. Formats: F7.3 latitudes/longitudes/pressure values. Size of data base ~ 500 Kb.
Other Remarks	Cloud–top pressure values are extracted using “nearest neighbour” as selection criterion but can optionally be interpolated in space and time. Application of bilinear interpolation in space and linear interpolation in time is controlled by a logical flag in the static initialisation file.

4.5.3 PMD threshold data base

Type of Data Base	Cloud
Name of Data Set	Reflectance thresholds for PMD–based cloud clearing algorithm
Description	Reference angles (zenith cosines), PMD clear–sky reflectance thresholds for three PMD’s and three surface types (black, sand, vegetation), respectively. Simulated apparent pressure and simulated thresholds at 758nm.
Dimensions/Size	4 angles and 3 x 3 x 4 threshold values. 4 x 15 apparent pressure values, 4 x 15 simulated threshold values.
Physical Units	Pressure values in hPa. Threshold values dimensionless.
Errors	unknown.
Reference Source	[A15]
Remarks on Usage	Not used operationally.
Control Selection	Automatic.
Data Library	GTHRESHLIB.f
Software Format	ASCII real numbers. Format of angles is F5.2, threshold reflectances in F5.3, apparent pressure in F7.1, simulated thresholds in F5.3. Size of data base is 1.43 kB.
Other Remarks	It was already suggested by the authors to include an algorithm to update the reflectance threshold values dynamically. This has never been carried out.

4.6 AMF multiple scattering correction LUT

Type of Data Base	AMF
Name of Data Set	Multiple scattering correction factors.
Description	Multiple scattering correction factors are required to overcome the lack of a fast enough operational RTM with full multiple scattering capability that is able to calculate on–line the required multiple scattering AMFs. Instead, correction factors (fitting coefficients) are stored for two molecules (O ₃ , NO ₂) at two wavelengths (325 nm, 437.5 nm) as function of albedo, height above sea level, and climatological zones (± 85 , +50, ± 35 , ± 10 , –60 deg.). Two tables have been created for normal view mode (LOS < 35 deg) and polar view mode (LOS > 35 deg) of GOME, respectively.
Dimensions/Size	Reference grids for 4 albedo values, 7 height values, 8 latitude zones. Coefficients are available for two view modes, two molecules and two wavelengths, 14 climatological zones (4 belts x 2 seasons x 2 hemispheres – 2 = 14, no seasons in the tropical belt), all height/albedo combinations, and 6 x 4 sun zenith/line–of–sight zenith angle fitting (2 x 2 x 2 x 14 x 4 x 7 x 6 x 4 = 75264 points) coefficients.
Physical Units	Height in km, latitudes in deg., wavelength in nm, all other quantities are dimensionless.
Errors	<i>a priori</i>
Reference Source	LUT created using GOMETRAN ([A36])
Remarks on Usage	AMFs are calculated from the stored coefficients for the given geolocation/geometry, height and albedo. First, correction factors are restored from the data base entries (by applying the initial fitting algorithm in reverse order); then Akima–interpolation is carried out over albedo, height and latitude zone (using cosines of latitudes for the latter) to derive the final correction factor.
Control Selection	Automatic.
Data Library	GMSCORRLIB.f
Software Format	ASCII double precision numbers for coefficients, real numbers for reference grids. Size of data set 603.008 Kb.
Other Remarks	The first polynomial fitting is carried out over the sun zenith angle (for all line–of–sight angles). In a second step, the fitting parameters from the previous fit are fitted over the line–of–sight angle. Fitting coefficients have been derived using singular value decomposition. MPI T–p–conc profiles [A4] were used and Mie phase functions were applied for aerosol scattering at a visibility of 23 km. 'Rural' aerosol is present in latitude bands +50, +35 deg while 'maritime' aerosol is present for all other latitude bands, reflecting the dominating surface type in the latitude belt. Note, that now only NO ₂ correction factors are in operational use for generating NO ₂ AMFs. Ozone AMFs were calculated in full multiple scattering mode using LIDORT [A44] and are now restored by neural networks.

Appendix A Auxiliary Data Bases

Compilation of auxiliary data bases not essential to GDP, but used in the scientific environment for test purposes and further development. No special order is given.

Rayleigh scattering

Type of Data Base	Aerosol
Name of Data Set	Rayleigh Scattering Correction
Description	Coefficients of pure rayleigh–scattered TOA intensities that are used to compute the Absorbing Aerosol Indicator (AAI).
Dimensions/Size	Reference grids for 2 wavelengths, 8 albedos, and 11 ground heights. Fitting parameters (coefficients) of a quasi–two–dimensional polynomial fit stored for 3 harmonics. Fitting parameters are derived as function of sun zenith angle and line–of–sight angle. The azimuth dependency of rayleigh backscatter intensities is taken into account using the harmonics. Polynomials of degree 5 and 3 (6 and 4 coefficients) have been used to fit for the sun zenith and line–of–sight angle, respectively First harmonic (nadir part) available for all variables mentioned above (2 x 8 x 11 x 6 x 4 = 4224 points). Harmonics 2 and 3 available for two wavelengths, 11 heights (2 x 11 x 6 x 4 = 528 points).
Physical Units	Reference wavelengths in nm. Albedo dimensionless, heights in km, fitting coefficients dimensionless.
Errors	<i>A priori</i>
Reference Source	AAI–algorithm: [A16] LUT created by R. Spurr using GOMETRAN.
Remarks on Usage	Used in the Absorbing Aerosol Indicator Algorithm that is not called during operational processing.
Control Selection	Computation of Absorbing Aerosol Index controlled by a logical flag. Usage of data base automatically.
Data Library	GRAYLUT.f
Software Format	ASCII real numbers. Formats: albedo in F5.2, height in F4.1, wavelength in F6.1, fitting parameters in 1PE14.7. Size of data set 43.186 Kb.
Other Remarks	Validation of AAI results required. Delivery of results to the public requires a change of the L2 product. Currently, no internal link to other algorithms (stand–alone result) and no link to aerosol optical depth. The first polynomial fitting is carried out over the sun zenith angle (for all line–of–sight angles). In a second step, the fitting parameters from the previous fit are fitted over the line–of–sight angle. Fitting coefficients have been derived using singular value decomposition.

Special Scenarios

Type of Data Base	Profile
Name of Data Set	Special Scenario Profiles
Description	Selected atmospheric and trace gas concentration profiles for several special scenarios: Ozone hole (day–time and night–time), Biomass burning, Volcanic, Polar Stratospheric Clouds, Industrial pollution, Twilight, "Worst Case".
Dimensions/Size	8 scenarios. Each scenario comprises several columns, with 201 entries in each column. The first column is altitude from 0.0 km to 100 km (resolution 0.5 km). Other columns may be temperature, aerosol extinction profiles at 550 nm (where applicable), or trace gas concentration profiles (choice of species depends on scenario).
Physical Units	Temperatures in degrees K. Trace gas concentrations as number mixing ratios. Aerosol extinction profile in km^{-1} .
Errors	<i>A priori</i>
Reference Source	See Appendix B.
Remarks on Usage	Climatological profile inputs to radiative transfer models (including AMF). Not designed to be used operationally – for test scenarios only.
Control Selection	Discretion in scientific testing and scenario investigation.
Data Library	PROFILES.PAR
Software Format	ASCII real numbers. Formats: heights F5.1, temperatures F8.3, all profiles 1PE11.5. Size of data set 29.748 Kb.
Other Remarks	Where experimental values are only available for a restricted altitude range they are supplemented by the appropriate profiles from the MPI database (smooth matching!). For trace gases not requiring special consideration, the MPI background data are used. Temperature and pressure profiles are also taken from this database unless indicated otherwise. See Appendix B for details.

Cloud scattering properties

Type of Data Base	Cloud
Name of Data Set	Cloud scattering
Description	Reference wavelength grid, cloud extinction, single scattering albedo, phase functions, phase function moments.
Dimensions/Size	Information for 5 standard low cloud types, 3 standard high cloud types (Stephens classification, see below). 25 wavelengths between 200 nm and 800 nm, extinction coefficients for 25 wavelengths and 8 cloud types, single scattering albedos for 25 wavelengths and 8 cloud types, phase functions between 0 and 180 degrees (1 deg. resolution) for each wavelength and cloud type, phase function moments (299) for each wavelength and cloud type
Physical Units	Extinction coefficients in km^{-1} . Wavelength grid in nm, phase function values in $(\text{Steradian})^{-1}$; all phase functions are normalised to 1. Phase function moments dimensionless.
Errors	unknown
Reference Source	[A47]
Remarks on Usage	Discretion: option exists to use data in AMF algorithm, but at present, this is not taken up. Phase function moments also used in GOMETRAN. [The problem here is that not enough information can be extracted from stand-alone GOME measurements to make the treatment of clouds as particle layers worthwhile on a routine operational basis.]
Control Selection	Usage of cloud information for AMF calculation controlled by a logical flag.
Data Library	GCLOUDLIB.f
Software Format	ASCII real numbers. Format of wavelengths is F6.1, extinction coefficients, single scattering albedos, phase functions and phase function moments stored as E11.5.
Other Remarks	This data base contains the results of the MIE calculations of phase functions and their moments, plus extinction coefficients and single scattering albedos, for the eight water-droplet clouds measured by Stephens. The Mie code is that due to Wiscombe. The following cloud types are available: <ol style="list-style-type: none">1. Stratus I (St I)2. Stratus II (St II)3. Stratocumulus I (Sc I)4. Stratocumulus II (Sc II)5. Nimbostratus (Ns)6. Altostratus (As)7. Fair Weather Cumulus (Cu)8. Cumulonimbus (Cb)

Lowtran sun spectrum

Type of Data Base	Spectroscopic
Name of Data Set	Sun reference spectrum (Lowtran)
Description	Wavelengths and Solar irradiance data
Dimensions/Size	2910 points for wavelengths and irradiances from 173.943 – 352.113 nm and 1241 points for wavelengths and irradiances from 347.464 – 2512.563 nm. Total entries are $2 \times 4151 = 8302$.
Physical Units	photons / (nm s cm ²)
Errors	see [A23] and references therein
Reference Source	LOWTRAN7 solar irradiance data; compiled from LOWTRAN 7 software package ([A22]).
Functional Usage	Used as external reference spectrum in DOAS fitting algorithm for test purposes and for simulating (absolute) radiance spectra at top of the atmosphere by means of a radiative transfer model. Not used operationally.
Control Selection	Presence of the external solar reference spectrum is controlled by a logical flag.
Data Library	GSUNLIB.f
Software Format	ASCII real numbers. Format F9.4 wavelengths, 1PE14.7 pseudo-cross-sections. Size of entire data base 602.126 Kb.
Other Remarks	

Anderson sun spectrum

Type of Data Base	Spectroscopic
Name of Data Set	Sun reference spectrum (Anderson)
Description	Wavelengths and Solar irradiance data
Dimensions/Size	11001 points for wavelengths and irradiances from 200.00 – 310.000 nm. Total entries are $2 \times 11100 = 12200$.
Physical Units	photons / (nm s cm ²)
Errors	unknown
Reference Source	G.P. Anderson solar irradiance data, [A23].
Functional Usage	Used as external reference spectrum in DOAS fitting algorithm and for simulating (absolute) radiance spectra at top of the atmosphere by means of a radiative transfer model. Not used operationally.
Control Selection	Presence of the external solar reference spectrum is controlled by a logical flag.
Data Library	GSUNLIB.f
Software Format	ASCII real numbers. Format F9.4 wavelengths, 1PE14.7 irradiances. Size of entire data base 602.126 Kb.
Other Remarks	

Combined Anderson/Kurucz sun spectrum

Type of Data Base	Spectroscopic
Name of Data Set	Sun reference spectrum (combined)
Description	Wavelengths and Solar irradiance data
Dimensions/Size	60000 points for wavelengths and irradiances from 200.00 – 799.99 nm. Total entries are 2 x 60000 = 120000.
Physical Units	photons / (nm s cm ²)
Errors	unknown
Reference Source	Robert Kurucz (SAO) and Hall and Anderson (AFGL) solar irradiance data, [A22].
Functional Usage	Used as external reference spectrum in DOAS fitting algorithm and for simulating (absolute) radiance spectra at top of the atmosphere by means of a radiative transfer model. Not used operationally.
Control Selection	Presence of the external solar reference spectrum is controlled by a logical flag.
Data Library	GSUNLIB.f
Software Format	ASCII real numbers. Format F9.4 wavelengths, 1PE14.7 irradiances. Size of entire data base 602.126 Kb.
Other Remarks	Solar irradiance data, combining data from Robert Kurucz (SAO) and from Hall and Anderson (AFGL). Note, that the combined spectrum is not an extraterrestrial spectrum but includes atmospheric absorption. Hall and Anderson data range: 200–310 nm Kurucz data range: 293.01–1626.5 nm

Oxygen spectroscopic data

Type of Data Base	Spectroscopic
Name of Data Set	O₂ Spectroscopic Line Data
Description	Exponential sum fitting coefficients in the Oxygen A band (centered around 760 nm).
Dimensions/Size	132 wavelength pairs (start and end wavelength), reference pressure (6) and reference temperature (5) grid, exponential sum fitting weights (10) and exponential sum fitting coefficients (132 x 6 x 4 x 10).
Physical Units	wavelength in nm, pressure in hPa, esft-coefficients in $\text{cm}^2 \cdot \text{mol}^{-1}$
Errors	unknown
Reference Source	[A5], based on HITRAN [A34] spectroscopic data.
Remarks on Usage	No direct application in operational Level 1 to 2 processing, but data can be used in RTM's for creating optical depths in the Oxygen A band.
Control Selection	Automatic.
Data Library	GO2A_ESFTLIB.f
Software Format	ASCII double precision numbers. Format F12.5 line positions (wavelength), D12.6 reference pressure, D12.6 reference temperature, D12.6 esft-weights, D13.5 esft-coefficients. Size of data set 256.530 kB.
Other Remarks	

Appendix B Notes on Special Scenarios for GOME

compiled by D. Diebel, IFE, Bremen

Eight different "special" scenarios have been created for the testing of GOME forward models and retrieval algorithms (there are two ozone hole scenarios). Wherever possible, information from the literature has been used. However, the "worst case" scenario is not very likely to occur; it compounds an ozone hole situation with PSCs, tropospheric pollution and volcanic particle loading. It should represent the worst case for Ozone retrieval. The scenarios have been compiled for testing purposes and should not be used in the operational Level 1 to 2 processing.

In the cases where experimental values are available only for a restricted altitude range, they are supplemented by the appropriate profiles from the MPI database. For trace gases with no special consideration, the MPI background data are used. Temperature and pressure profiles are also taken from this database unless indicated otherwise.

The scenarios are available on floppy, and have been incorporated into the GOMEware. In the data base, altitudes are in [km], mixing ratios in [ppm] for trace gases, the extinction coefficient at 550 nm in [km^{-1}] for aerosols, and temperatures in [K].

1. Ozone Hole (Daytime)

Latitude: 81° S
Month: October
Solar zenith angle: 80°
MPI profile: 85° S, October

O₃:

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al. (J. Geophys. Res. 94 D9, 11,429, 1989). Ground level assumed at 3 km. Depletion in O₃ follows approximately Gaussian profile, centred at 20 km altitude with a halfwidth 8 km. This is used to correlate other gases.

NO₂:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 0.5 ppb, subtracted from MPI profile. This reduces the background column density of 3.2×10^{16} molecules/cm² to 2.3×10^{16} molecules/cm². This in agreement with Sanders et al. (J. Geophys. Res. 94 D9, 11,381, 1989) and Solomon and Keys (J. Geophys. Res. 97 D8, 7971, 1992) stating strongly decreased values between August and mid September during the vortex, which are nearly back to normal in October.

ClO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 1 ppb, added to MPI profile. Taken from papers by Brune et al. (J. Geophys. Res. 94 D14, 16,649, 1989) and Zafra et al. (J. Geophys. Res. 94 D9 11,423, 1989).

BrO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 10 ppt, added to MPI profile. From Solomon et al. (J. Geophys. Res. 92 D7. 8329, 1987).

T:

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al.

2. Ozone Hole (Night)

Latitude: 81° S

Month: October

Solar zenith angle: 93°

MPI profile: 85° S, October

O₃:

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al. (J. Geophys. Res. 94 D9, 11,429, 1989). Ground level assumed at 3 km. Depletion in O₃ follows approximately Gaussian profile, centred at 20 km altitude with a halfwidth of 8 km. This is used to correlate other gases.

NO₂:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 0.5 ppb, subtracted from MPI profile. This reduces the background column density of 3.2×10^{16} molecules/cm² to 2.3×10^{16} molecules/cm². This in agreement with Sanders et al. (J. Geophys. Res. 94 D9, 11,381, 1989) and Solomon and Keys (J. Geophys. Res. 97 D8, 7971, 1992) stating strongly decreased values between August and mid September during the vortex, which are nearly back to normal in October.

ClO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 1 ppb, added to MPI profile. Taken from papers by Brune et al. (J. Geophys. Res. 94 D14, 16,649, 1989) and Zafra et al. (J. Geophys. Res. 94 D9 11,423, 1989).

OCIO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 5 ppt, added to MPI profile. Results in column content of 2.6×10^{13} molecules/cm², which is about a factor of 2 higher than experimental data (e.g., Sanders et al., J. Geophys. Res. 94 D9, 11,381, 1989). On the other hand, the column density given by the MPI profile (which does not model ozone depletion processes) is already 1.7×10^{13} molecules/cm². Comments, please!

T:

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al.

3. Tropospheric Industrial Pollution

Latitude: 52° N

Month: January

Solar zenith angle: 75°

MPI profile: 55° N, January

O₃: Constant value of 100 ppb in planetary boundary layer between 0 and 1.5 km, based on various experimental data (e.g., Browell, Proc. IEEE 77, 419, 1989; Smit et al., Berichte des Forschungszentrums Jülich 2568, 1991).

NO₂:

10 ppb between 0 and 1.5 km. In agreement with Fricke (Luft kennt keine Grenzen, Umweltbundesamt, 1991).

HCHO:

5 ppb between 0 and 1.5 km.

SO₂:

100 ppb between 0 and 1.5 km. Corresponds to winter smog condition (Fricke, Luft kennt keine Grenzen, Umweltbundesamt, 1991). It is arguable whether GOME will ever see an average concentration of 100 ppb within its ground pixel of 320 km by 40 km. Comments!

Aerosol:

LOWTRAN urban aerosol in boundary layer with 2 km visibility. Above LOWTRAN background aerosol for fall/winter condition with visibility of 23 km in troposphere.

4. Biomass Burning Pollution

Latitude: 4° N

Month: January

Solar zenith angle: 35°

MPI profile: 5° N, January

O₃:

Two Gauss profiles added to MPI profile. First one centred at 2.5 km, halfwidth 1.5 km, the other centred 7.5 km, halfwidth 1.5 km. Peak values such that addition to MPI profile models experimental data by Marenco et al. (Atmos. Environ. 24A, 2823, 1990) with peak values of 100 ppb.

NO₂:

Two Gauss profiles, correlated to O₃, with peak values of 10 ppb added to MPI profile. Values in agreement with Burrows et al. (Meteorfahrt, BMFT Report).

HCHO:

Two Gauss profiles, correlated to O₃, with peak values of 5 ppb added to MPI profile. Values in agreement with Burrows et al. (Meteorfahrt, BMFT Report).

Aerosol:

Two Gauss profiles, correlated to O₃, added to LOWTRAN background aerosols for fall/winter with visibility of 23 km in troposphere. Peak extinction at 550 nm is about 0.2 km⁻¹ at 2.5 km altitude (background 0.05 km⁻¹) and 0.1 km⁻¹ at 7.5 km (background 0.002 km⁻¹)

T:

Smoothed experimental data by Marenco et al. (Atmos. Environ. 24A, 2823, 1990).

5. Polar Stratospheric Clouds

Latitude: 72° S

Month: August

Solar zenith angle: 90°

MPI profile: 75° S, August

NO₂:

NO₂ is usually depleted during the antarctic winter season. This is reflected by the MPI database, which shows a sharp increase in NO₂ between September and October. In August, the MPI column density is about 4.4 x 10¹⁵ molecules/cm².

Aerosol:

LOWTRAN background aerosol for fall/winter with 50 km visibility in troposphere with added Gauss peak, centred at 17 km, halfwidth 2 km, with a peak value of about 0.02 km⁻¹ extinction at 550 nm. The chosen thickness and extinction are typical for PSCs (e.g., Kinne et al., Geophys. Res. Lett. 17, 2079, 1990; Torres et al., J. Geophys. Res. 97 D12, 13,015, 1992).

6. Twilight

Latitude: 65° S

Month: January

Solar zenith angle: 93°

MPI profile: 65° S, January

NO₃:

Typical profiles can be found in Wayne et al. (The Nitrate Radical, Air Poll. Res. Rep. 31, Comm. European Communities, 1990). The profile used is a digitization of Fig. V14.

7. Volcanic Eruption

Latitude: 4° N

Month: September

Solar zenith angle: 20°

MPI profile: 5° N, September

Aerosol:

LOWTRAN background aerosol for fall/winter between 0 and 10 km with a visibility of 23 km. Between 10 and 30 km LOWTRAN extreme volcanic aerosol for fall/winter, featuring a peak at 18 km with about 3 km halfwidth. The peak extinction at 550 nm is 0.1 km^{-1} . Above 30 km LOWTRAN mesospheric with transition from extreme volcanic.

SO₂:

Gauss profile, centred at 18 km, halfwidth 3 km, added to MPI profile. The value in the maximum is 70 ppb, which is derived from experimentally observed total columns of about 5×10^{16} molecules/cm² (Goldman et al., Geophys. Res. Lett. 19, 179, 1992).

NO₂:

Gauss profile, centred at 18 km, halfwidth 3 km, with peak value of 0.1 ppb subtracted from MPI profile. This leads to values of zero for NO₂ between 15.5 and 18.5 km. Experiments indicate a loss of 20 to 40% in column density (e.g., over Lauder, New Zealand, Johnston et al., Geophys. Res. Lett. 19, 211, 1992), but this cannot be realized for a volcanic cloud restricted to an altitude range of only 3 km.

8. Worst Case Scenario

Latitude: 81° S

Month: October

Solar zenith angle: 80°

MPI profile: 85° S, October

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al. (J. Geophys. Res. 94 D9, 11,429, 1989). Ground level assumed at 3 km. Identical to ozone hole scenario 1).

ClO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 1 ppb, added to MPI profile. Identical to ozone hole scenario.

BrO:

Gauss profile, centred at 20 km altitude, halfwidth 8 km, peak value 10 ppt, added to MPI profile. Identical to ozone hole scenario.

T:

Smoothed experimental data between 3 and 29 km for October 16, 1986 by Komhyr et al.. Identical to ozone hole scenario.

NO₂:

Gauss profile, centred at 18 km altitude, halfwidth 3 km, peak value 0.5 ppb, subtracted from MPI profile to take into account depletion by volcanic cloud. A value of 10 ppb for NO₂ is taken to represent a polluted troposphere between 0 and 1.5 km.

SO₂:

Gauss profile, centred at 18 km, halfwidth 3 km, added to MPI profile. The value in the maximum is 70 ppb. This value corresponds to the volcanic scenario. In addition, values in the boundary layer between 0 and 1.5 km are increased to 10 ppb, reflecting a tropospheric pollution.

HCHO:

Pollution levels of 5 ppb between 0 and 1.5 km.

Aerosol:

LOWTRAN urban aerosol in boundary layer with visibility of 2 km. Above LOWTRAN tropospheric background aerosol up to 10 km for a spring/summer condition, visibility 50 km. Above 10 km LOWTRAN volcanic aerosol for spring/summer with a peak at 20 km. A PSC is added at 17 km altitude identical to that in the PSC scenario.