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Impact of Using Different Ozone Cross Sections on Ozone Profile Retrievals from GOME Ultraviolet Measurements

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Abstract We investigated the effect of using three sets of different cross sections on ozone profile retrievals from GOME ultraviolet observations: Bass-Paur cross sections archived in HITRAN, Brion cross sections, and cross sections measured by the GOME flight model. Using different cross sections can significantly affect the retrievals, by up to 15 DU in total column ozone, by up to 10 DU tropospheric column ozone, and by up to 20-30% at individual layers. Compared to using the Bass-Paur and GOME flight model cross sections, the use of Brion cross sections not only leads to more successful retrievals and reduces the fitting residuals by 5-10% and 30-45% in the Hartley and Huggins bands, respectively, but also generally improves the retrievals especially in the troposphere. The retrieved total column ozone with the GOME flight model is systematically lower by 6-10 DU than with the Brion and Bass-Paur cross sections.

1. Introduction to Ozone Cross Sections

- Three ozone cross sections (Table 1) [Orphal, 2002]

Table 1. Measurement characteristics of Bass-Paur, Brion et al., and GOME Flight model cross sections.

	Bass-Paur	Brion et al.	GOME-FM
Instrument	scanning monochromator	Jobin Yvon THR1500 & 640 spectrometer	monochromator with 4 diode-array detectors
Wavelength (nm)	245-343	195-345[1]	231-794
Spectral Res. (nm)	0.025	0.01	0.2-0.4
Temperature (K)	203, 218, 228, 243, 273, 298	218, 228, 243, 273, 295	202, 221, 241, 273, 293
Data Sampling (nm)	0.05[2]	0.01	GOME wavelength grid
References	Bass & Paur, 1981, 1985 Paur & Bass, 1985	Daumont et al.,1992 Brion et al,1993 Malicet et al.,1995	Burrows et al., 1999

1. 300-345 nm for 273 k 2. Quadratic coefficients at each wavelength

- Orphal [2002] critically reviewed these cross sections and found that:
  - The agreement between these measurements is generally 1-2% in the Hartley and Huggins bands after wavelength shifts.
  - The Brion et al. data are less noisy and have more accurate wavelength calibration, but does not cover below 218 k.
- The Bass-Paur data are widely used in the scientific community and are included in HITRAN [Orphal and Chance, 2003]
- The GOME FM data are used for GOME DOAS operational total O_3 retrieval and O_3 profile retrieval by Hoogen et al. [1999].

2. Motivation

- What is the effect of using these "close" cross sections on ozone profile retrievals?
- Which one should be used for ozone profile retrievals from UV measurements?

3. Methodology

- Use exactly the same retrieval algorithm and input parameters (other than ozone cross sections) except that Bass-Paur and Brion et al. cross sections are convolved to the GOME spectral resolution.
- Derive quadratic fitting coefficients for Brion et al. and GOME FM data using NLLS fitting.
- Wavelength shifts between ozone cross sections and radiances are fitted on line with a 3rd-order polynomial
- Compare retrievals of several orbits and data overpass the Hohenpeißenberg ozonesonde/Dobson station during 1997.

4. Ozone Profile Retrieval Algorithm

- Optimal estimation + spectral fitting (289-307 nm, 325-338 nm) [Liu et al., 2005]
- Derive partial column ozone at 24 layers (each layer is ~2.5 km) from surface to ~60km
- A priori ozone profile climatology from 15 years of SAGE, ozonesonde and MLS by McPeters et al. [2003]
- Wavelength and radiometric calibrations
- Accurate forward modeling of atmospheric state (GOMECAT clouds, NCEP surface/tropopause pressure and temperature profiles, GEOS-CHEM aerosols fields, SAGE background aerosols, GOME albedo database, NO_2, BrO, SO_2, and HCHO) with LIDORT and other corrections (e.g., Ring effect and polarization correction) [Liu et al., 2005]

5. Comparison of Various Retrievals

- Smaller Fitting residuals with the Brion cross sections: by 5-10% in the 289-307nm, by 30-45% in 325-338 nm. Similar fitting residuals between with Bass-Paur & GOME FM data (Fig. 1, Table 2)
- More successful retrievals with the Brion et al. cross sections (Table 2)
- The retrieved total column ozone with the GOME FM is smaller by 5-15 DU than with the other two (Fig. 2), smaller by 7-10 DU on average (Table 2).

Table 2 Comparison of # of retrievals, fitting residuals, Total Column Ozone (TCO), and Tropospheric Column Ozone (TRCO) for two orbits of retrievals and GOME overpass over Hohenpeißenberg in 1997.

Orbit/Station		Brion	BP	GM FM
70607024	n_{ret}	**201**	196	200
	res_{ch1} (%)	**0.358**	0.384	0.382
	res_{ch2} (%)	**0.082**	0.127	0.129
	TCO (DU)	304.6	303.5	**295.6**
	TRCO (DU)	30.4	27.8	26.7
61201030	n_{ret}	**192**	167	197
	res_{ch1} (%)	**0.345**	0.368	0.373
	res_{ch2} (%)	**0.082**	0.123	0.125
	TCO (DU)	283.5	282.8	**276.0**
	TRCO (DU)	24.8	22.9	21.3
Hohenpei-ßenberg(1997)	n_{ret}	**235**	233	201
	res_{ch1} (%)	**0.340**	0.379	0.377
	res_{ch2} (%)	**0.077**	0.144	0.134
	TCO (DU)	319.9	318.2	**308.7**
	TRCO (DU)	33.0	28.3	32.1

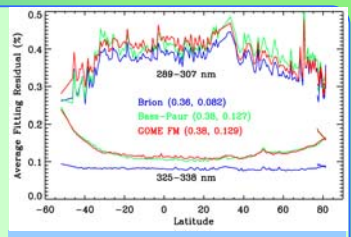

Fig. 1 Average fitting residuals in 289-307nm & 325-338 nm for orbit 70607024.

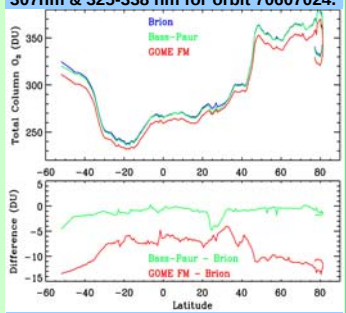

Fig. 2 Comparison of retrieved total column ozone for orbit 70607024.

- Retrieved Tropospheric Column Ozone (TRCO) can differ by up to 10 DU(30%) (Fig .3). TRCO with Bass-Paur & GOME FM is smaller by 1-5 DU on average than that with the Brion data.
- Profile differences of up to ~20% occur in the troposphere (GOME FM/Bass-Paur relative to Brion) and lower stratosphere (GOME FM relative to Brion/Bass Paur) (Fig. 4)

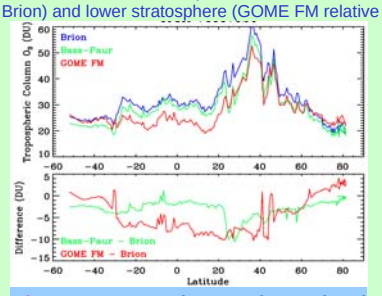

Fig. 3 Comparison of retrieved tropospheric column ozone for orbit 70607024.

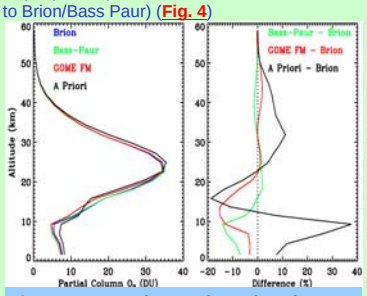

Fig. 4 Comparison of retrieved ozone profiles averaged over an orbit of retrievals (70607024).

6. Comparison of Various Retrievals with Coincident Observations

- TOMS: averaged over GOME footprint, < 1hr
- Dobson/sonde: <8º-lon, <1.5º-lat, < 8hrs, apply GOME averaging kernels to sonde measurements
- Retrievals shows smaller/slightly worse biases (1-4 DU)/standard deviations relative to TOMS/Dobson. Retrievals shows positive biases of 3-5 DU with Brion data and negative biases of 5-8 DU with GOME FM data (Fig. 5, Table 3).
- Retrievals with Brion data compares best with ozonesonde TRCO. Using Bass-Paur data leads to -4 DU bias in TRCO (Fig. 5, Table 3).
- Retrieved profiles can differ, on average, by up to 20-30% with different cross sections (Fig. 6).

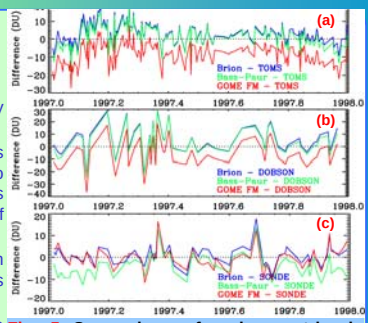

Fig. 5 Comparison of various retrievals with coincident observations: (a) TOMS TCO; (b) Dobson TCO; (c) Sonde TRCO.

Table 3 Comparison statistics (mean bias, 1σ, and correlation coefficient) between various retrievals and coincident observations over Hohenpeißenberg in 1997.

		Brion	BP	GMFM
TOMS TCO (n=175)	MB	2.8	1.3	-8.3
	1σ	5.8	5.9	5.8
	R	0.986	0.985	0.985
Dobson TCO (n=49)	MB	5.1	3.7	-5.8
	1σ	11.4	11.6	11.4
	R	0.946	0.944	0.945
Ozonesonde TRCO (n=66)	MB	0.46	-4.1	-0.45
	1σ	3.5	4.0	4.39
	R	0.757	0.771	0.691

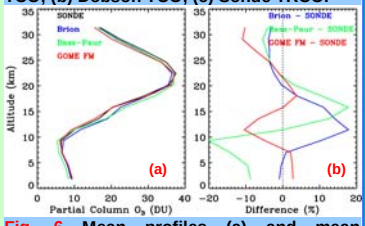

Fig. 6 Mean profiles (a) and mean differences (b) relative to sonde observations at Hohenpeißenberg in 1997.

Summary

- Investigate the impact of using different cross sections on GOME ozone profile retrievals
- Using different cross sections can significantly affect retrievals:
  - up to 15 DU in total column ozone (6-10 DU on average)
  - up to 10 DU in tropospheric column ozone (1-5 DU on average)
  - up to 20-30% at individual layers
- Using Brion cross sections leads to more successful retrievals and reduces fitting residuals by 5-10% and 30-45% in the Hartley and Huggins bands, respectively.
- Using Brion cross sections generally improves the retrievals especially in the troposphere
- Retrieved total column ozone with GOME FM are systematically lower by 6-10 DU.

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