Impact of ozone cross-section choice on (WF)DOAS total ozone retrieval

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Topics

- (WF)DOAS total ozone retrieval
- Direct comparisons of cross-sections
- Retrieval tests using different cross-sections

DOAS total ozone retrieval and ozone temperature

Weighting function DOAS

$$\ln \frac{I_{obs}}{F_{obs}} = \boxed{\ln\left(\frac{I}{F}\right)_{mod}} + \boxed{+\frac{d\ln(I/F)}{d\mathrm{TOZ}}\Big|_{mod}}(\mathrm{TOZ}_{fit} - \mathrm{TOZ}_{clim}) + \boxed{+\frac{d\ln(I/F)}{d\mathrm{T}}\Big|_{mod}}(\mathrm{T}_{fit} - \mathrm{T}_{clim}) + \ldots + \mathrm{Pol}$$

Radiation transfer model

Coldewey-Egbers et al., 2005

"Standard" DOAS

$$\ln \frac{I_{obs}}{F_{obs}} = -SC_1 \cdot \sigma(T_1) - SC_2 \cdot \sigma(T_2) + + \cdots + Pol$$

$$TOZ = (SC_1 + SC_2)/\boxed{AMF}$$

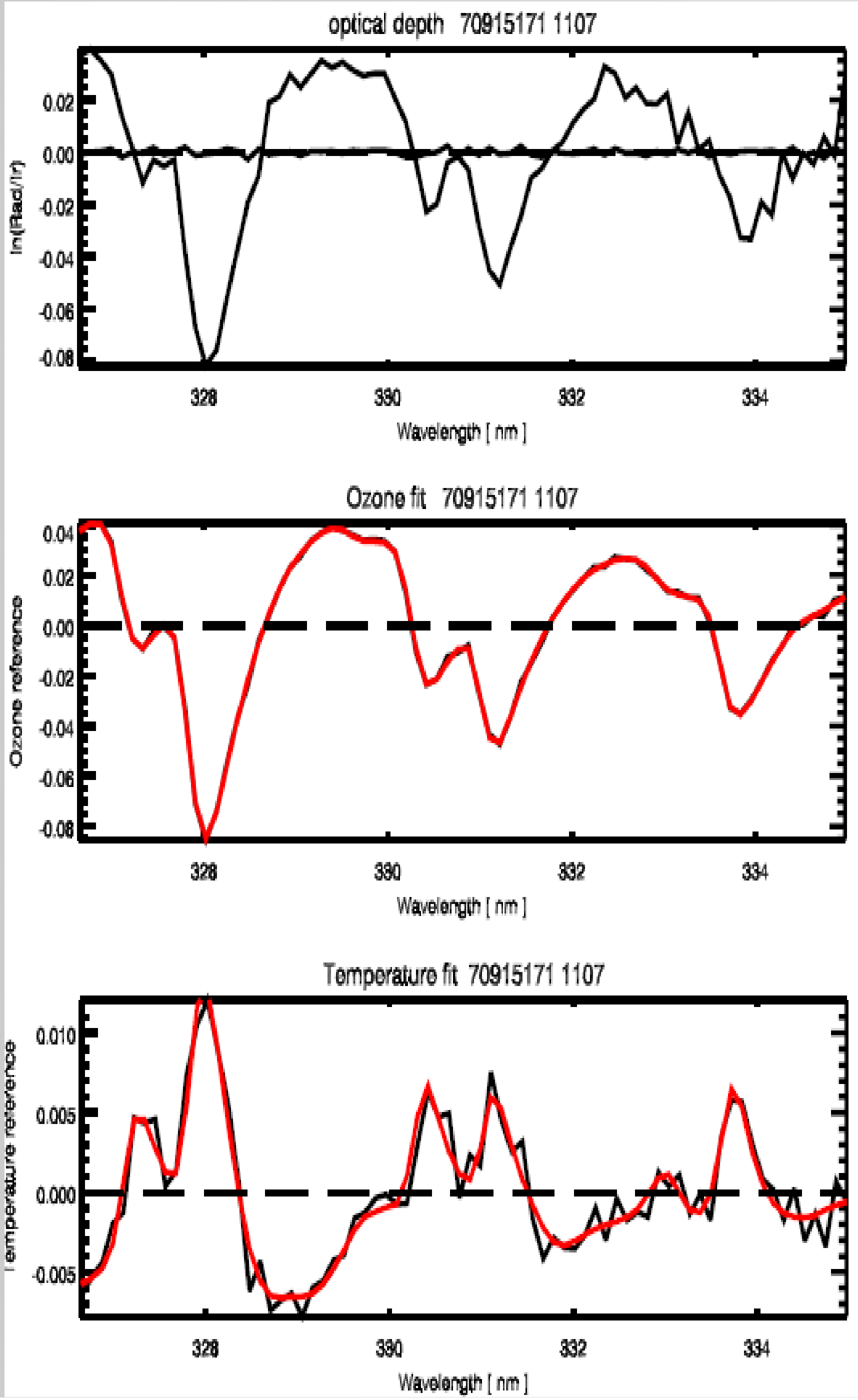
$T_1 \approx 220\,\mathrm{K}$
$T_2 \approx 240\,\mathrm{K}$

Radiation transfer model

Roozendael et al., 2006

➔ DOAS satellite retrievals

- 325-335 nm (WFDOAS: 336.6-335 nm)
- Weighting function DOAS (Coldewey-Egbers et al., 2005, Weber et al., 2005)
  - Scalar temperature shift in the a-priori temperature profile
- Standard DOAS: ESA operational retrieval (Roozendael et al. 2006)



Ozone and temperature terms in WFDOAS equation

- ▶Anti-correlation between ozone and ozone temperature term

- ▶Depending on fitting window size and position correlation ranges between r = -0.4 and -0.6

Coldewey-Egbers et al., 2005

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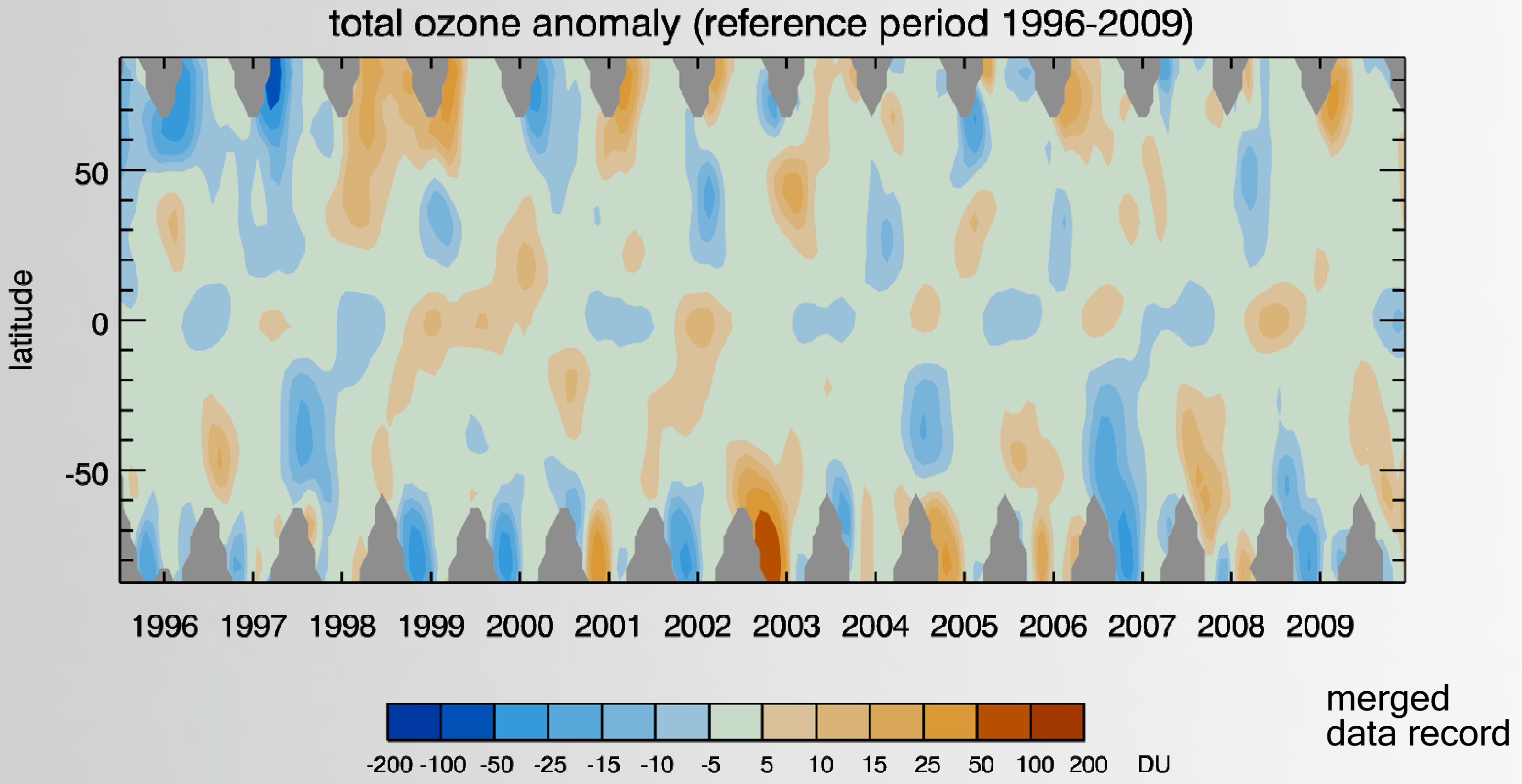
WFDOAS total ozone data sets/cross-section used

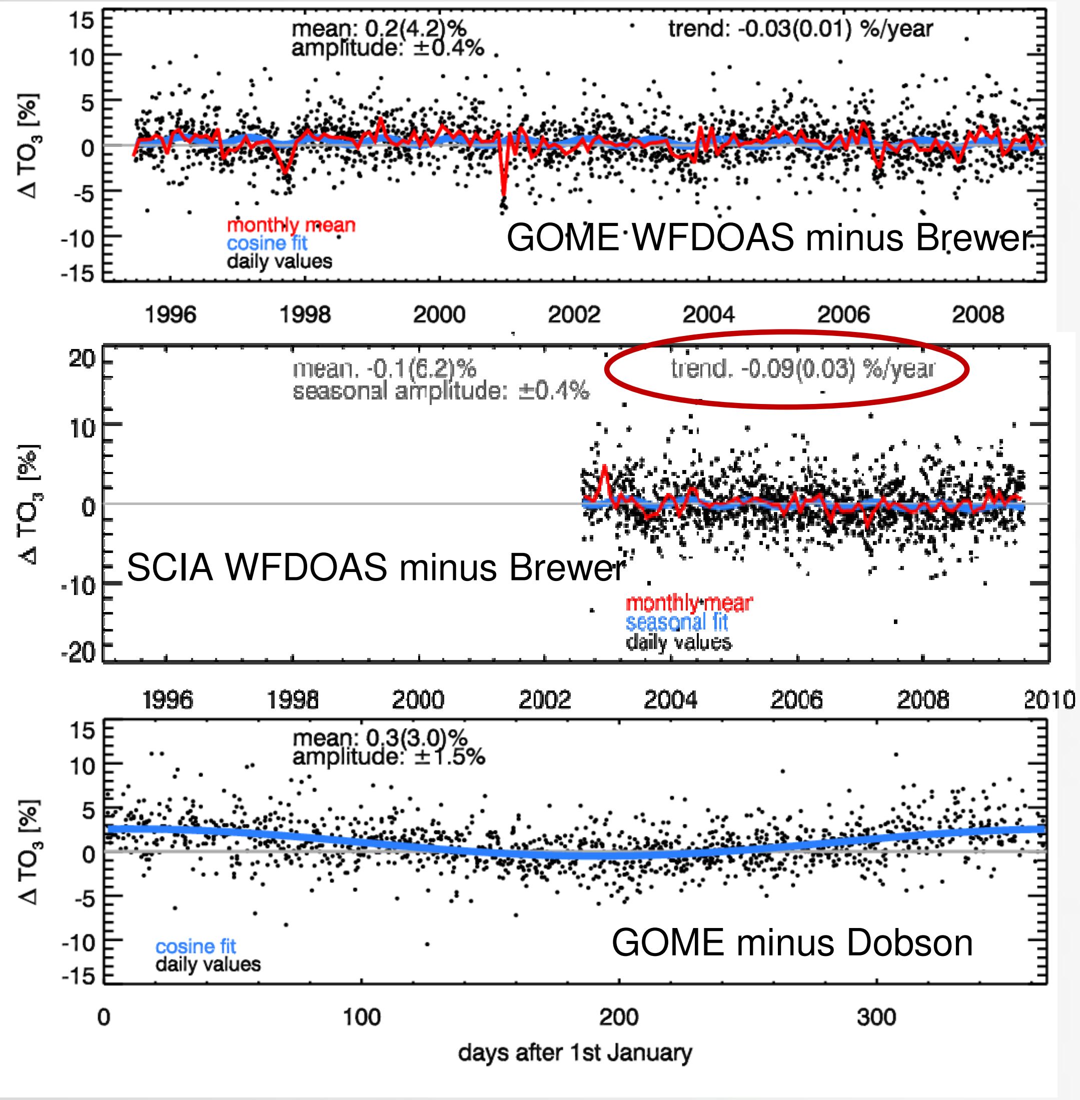


- WFDOAS applied to GOME (since 1995), SCIAMACHY (since 2002), and GOME2 (since 2006)
  - ➔GOME1/ERS : Burrows et al. 1999 (GOME FM), shift: +0.17 nm
  - ➔SCIAMACHY/ENVISAT Bogumil et al., 2003 (SCIA FM), scaled 5.3%, shift: +0.08 nm
  - ➔GOME2/METOP A: Burrows et al., 1999, convolved, shift: +0.017nm

GOME WFDOAS comparison to ground (at Hohenpeissenberg)

- Very good agreement, higher seasonality in the differences with Dobsons
- Error sources:
  - ➔ temperature dependence of cross-section (fixed T in ground retrievals)
    - Dobson error: 1.3%/10K (Komhyr et al. 1988)
    - Brewer error: 0.0-0.9%/10K (Kerr 2002)
  - ➔ Different x-sections
    - Bass-Paur (Brew/Dobs) vs. Burrows et al. (GOME)
  - ➔ Instrumental issues
    - straylight issue at high SZA (all instruments)
    - Calibration and optical degradation of satellite instruments (UV sensors)

Hohenpeissenberg 48°N,11°E



Cross-section data tested

- Ozone cross-section data
  - ➔ GOME FM (Burrows et al., 1999)
    - T=202 K, 221 K, 241 K, 273 K, 293 K
    - spectral resolution: 0.17 nm @ 330 nm
  - ➔ SCIAMACHY FM (Bogumil et al., 2003)
    - T=203 K, 223 K, 243 K, 273 K, 293 K
    - spectral resolution: 0.20 nm @ 330 nm
  - ➔ GOME2 FM3 V3 (Gür et al. 2005)
    - T=(203 K), 223 K, 243 K, 273 K, 293 K
    - spectral resolution: 0.29 nm @ 330nm

currently under revision

  - ➔ Bass-Paur (Paur and Bass, 1985)
    - T=203 K, 218 K, 228 K, 243 K, 273 K, 298 K
    - spectral resolution: ~0.05 nm(?)
  - ➔ Malicet et al. (1995), Brion et al., (1993), Daumont et al. (1998)
    - T=218 K, 228 K, 243 K, 273 K, 295 K
    - spectral resolution: 0.01-0.02 nm

- Temperature parametrerisation after Bass-Paur (t temperature in °C, λ wavelength in nm):

$$\sigma(\lambda, t) = a_0(\lambda)\left[1 + a_1(\lambda)t + a_2(\lambda)t^2\right]$$

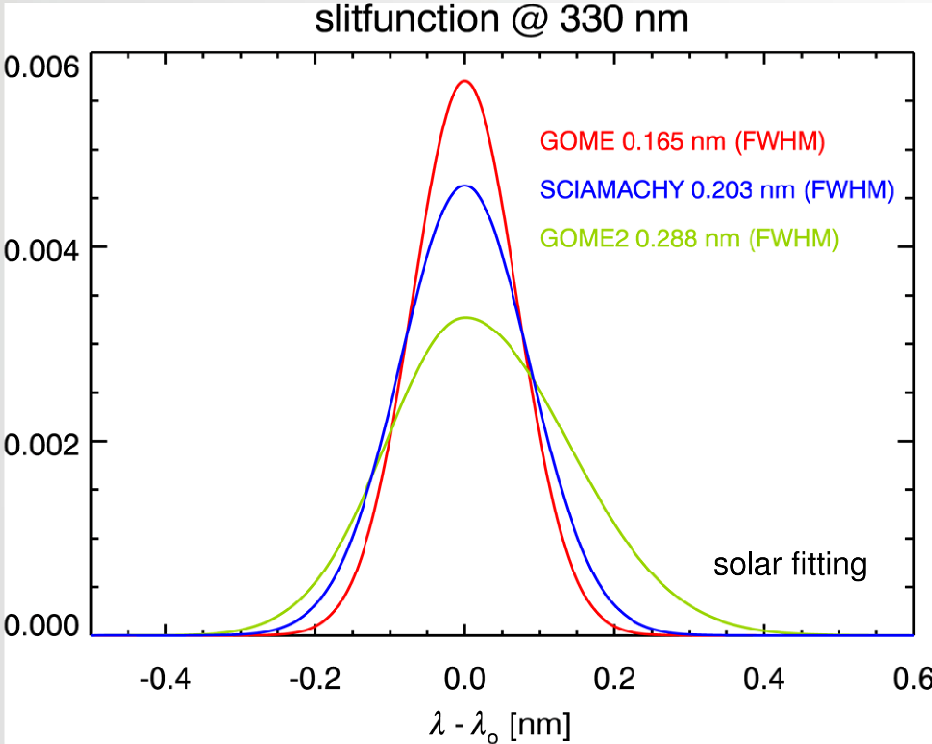
Direct comparisons of cross-sections/Solar fitting

- Slit function derived from comparison between (a) cross-sections and (b) from solar data

$$\sigma'(\lambda, T) = c_0 \cdot \sigma(\lambda + \Delta\lambda, T) \otimes r(\lambda) + Pol(\lambda)$$
$$I'(\lambda) = c_0 \cdot I(\lambda + \Delta\lambda) \otimes r(\lambda) + Pol(\lambda)$$

- Fit parameters in non-linear least squares fit:
  - ➔ Scaling factor: c_o
  - ➔ wavelength shift: $\Delta\lambda$
  - ➔ Instrument function r(λ)
  - ➔ Polynomial: *Pol(λ)*

- High spectral resolution reference data:
  - ➔ Kitt-Peak FTS solar data
  - ➔ Brion O3 cross-sections



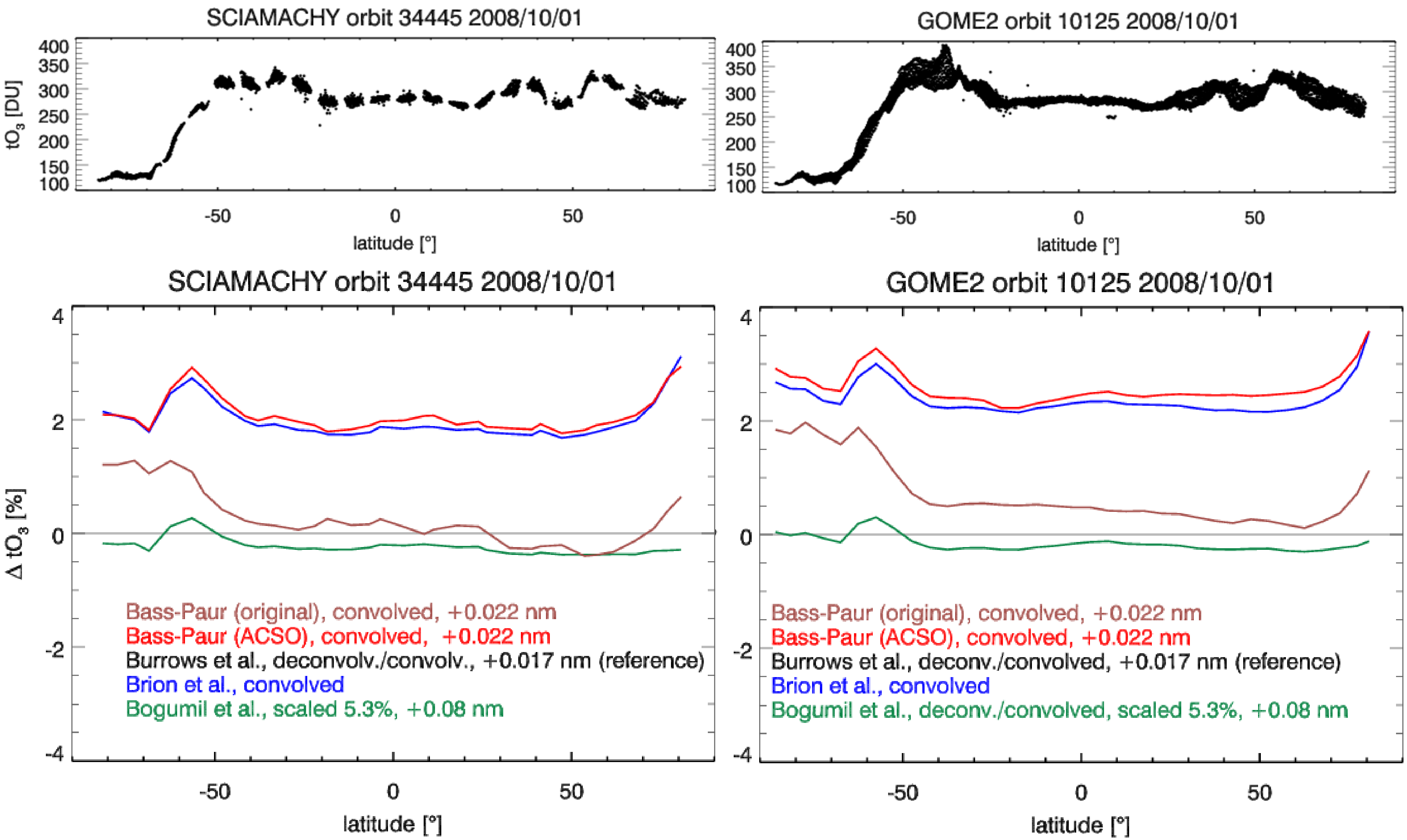
Cross-section issues in satellite DOAS I

Cross-sections	T[K]	Shift [nm]	Scaling [-]	Gaussian FWHM [nm]	Solar FWHM [nm]	Scaling wrt. GOME FM
Burrows et al. 1999 GOME FM	225 240	+0.017(2) +0.017(2)	1.027(2) 1.023(2)	0.158(5) 0.159(6)	0.165(8)	- -
Bogumil et al. 2003 SCIAMACHY FM	225 240	+0.008(2) +0.009(2)	0.970(3) 0.973(3)	0.222(6) 0.219(6)	0.202(13)	-5.6% -4.9%
Bass & Paur, 1985 (original, MPI database)	225 240	+0.020(3) +0.023(5)	1.015(3) 1.000(3)	0.079(10) 0.087(10)	-	+1.2% +2.3%
Bass & Paur, 1985 (ACSO web page)	225 240	+0.024(4) +0.021(4)	1.004(3) 1.004(3)	0.084(12) 0.078(11)	-	+2.3% +1.9%

Slitfunction fits w.r.t. Brion cross-sections: 326.6-334.5 nm

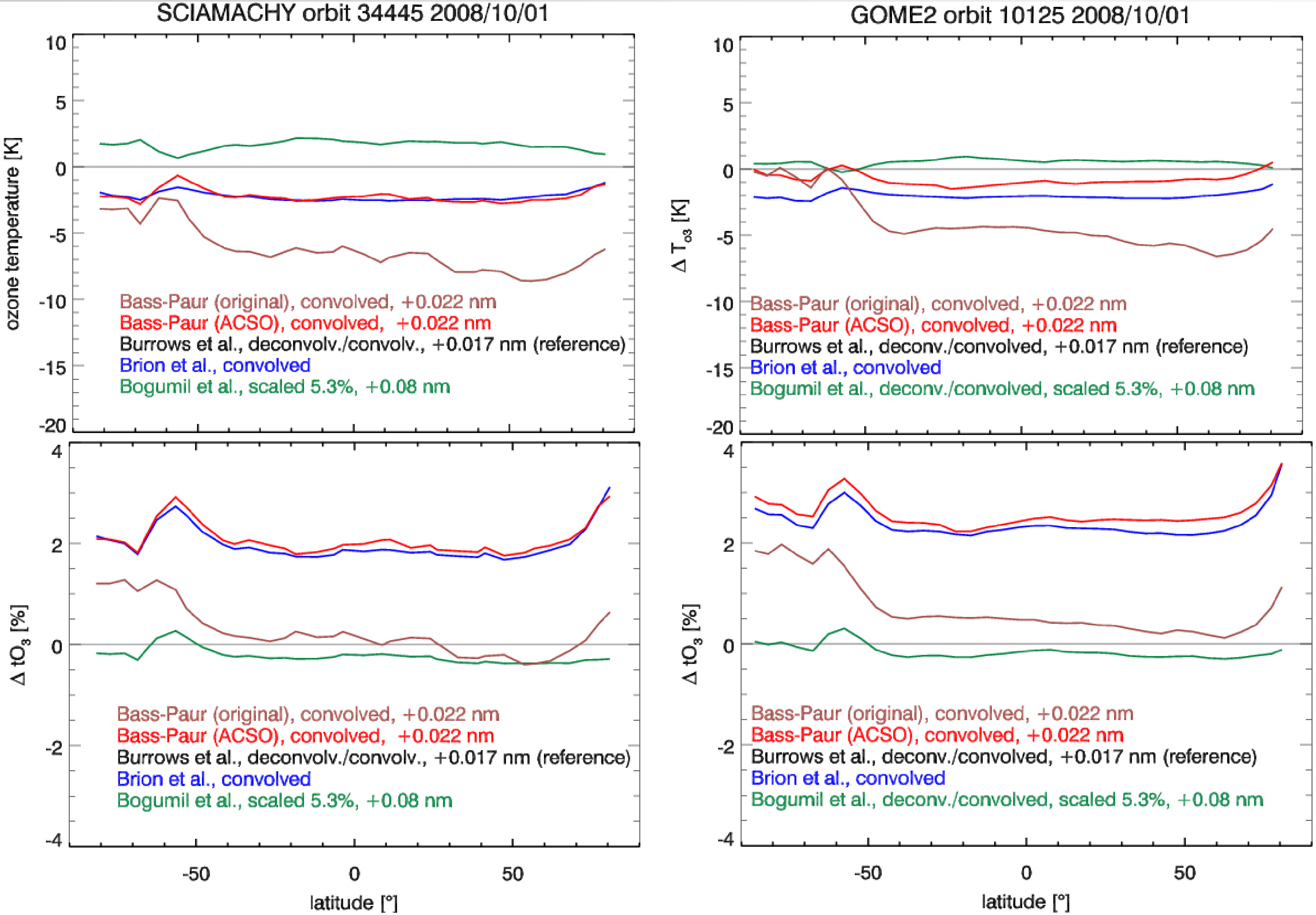
- Shifts minimising fit residuals in WFDOAS agree with shifts from cross-section comparisons (good wavelength calibration for Brion et al.)
- SCIAMACHY FM requires a scaling of +5% wrt to GOME1
- Note: total ozone change is -6DU/0.01nm shift (or -2%/0.01 nm) !!!

Retrieval test: SCIAMACHY & GOME2



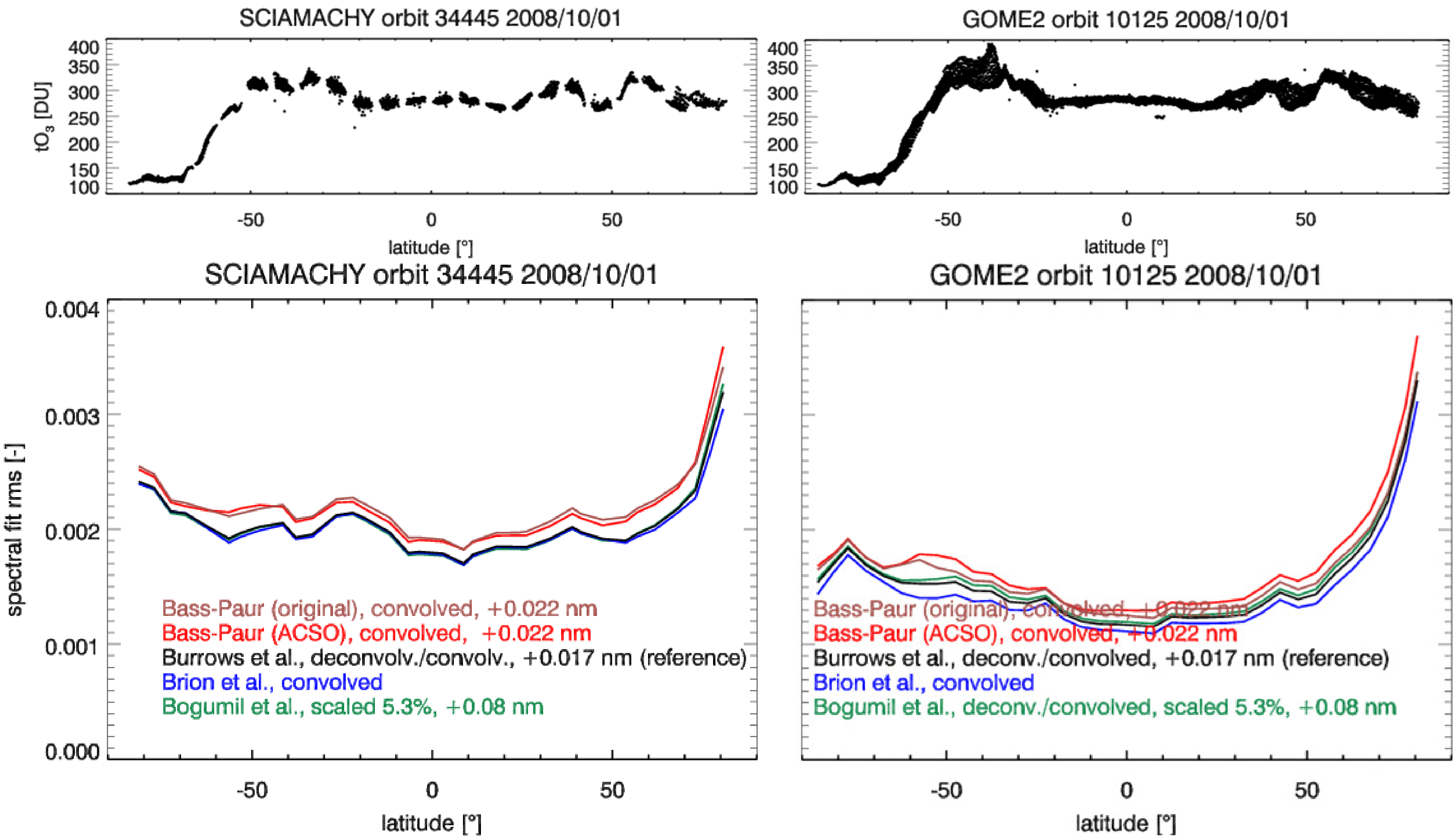
- Brion et al. & Bass-Paur (ACSO) ozone agree well and are 2-3% higher than SCIA/GOME-FM
- Using proper scaling for SCIA-FM, agreement with GOME-FM below 0.5%

retrieval test/ ozone temperature change



- Small changes in tO3 differences from SCIA to GOME related to changes in ozone temperature

Retrieval test/ spectral fit rms



- higher fit residuals with Bass-Paur
- Brion et al. similar (SCIA) or slightly lower (GOME2) than SCIA/GOME-FM

Summary and conclusion

- Comparison of different cross-sections used in satellite retrievals require
  - ➔ Proper wavelength shifts
    - ❍ direct comparison of cross-sections
    - ❍ verification by minimisation of spectral fit residuals
  - ➔ Proper scaling
    - ❍ direct comparison of cross-sections
    - ❍ Verification of scaling by retrieval comparisons
    - ❍ Some compensation/changes can occur due to interference of ozone and temperature terms in the (WF)DOAS equation

- Satellite DOAS ozone retrievals in the 325-335 nm window
  - ➔ Brion cross-sections are well wavelength calibrated (no shifts required)
  - ➔ Bass-Paur (ACSO) with shifts of 0.022 nm produces same results as Brion et al. but with higher spectral fit residuals
  - ➔ GOME-FM and scaled SCIA-FM (+5%) provide same ozone results, but use of Brion/Bass-Paur leads to differences of +2 to +3% in retrieved ozone
  - ➔ Fit residuals from Brion and GOME/SCIA-FMs are similar

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Requirements on „new" UV/Vis x-section measurements

- Important requirements for laboratory measurements
  - ➔ Wavelength calibration (-2% O3 error/0.01nm shift)
  - ➔ Absolute scaling, e.g. cross-path experiment with 253.65 nm as reference
  - ➔ Temperature stability & sufficient numbers of temperature points
  - ➔ Good slit function characterisation and/or sufficient high spectral resolution (~0.01 nm)
- ESA HARMONICS study
  - ➔ new cross-section measurements (talk by Anna Serdyuchenko)
  - ➔ Reanalysis of GOME, SCIA, and GOME2 x-section data