Impact of ozone cross-section choice on DOAS total ozone retrieval

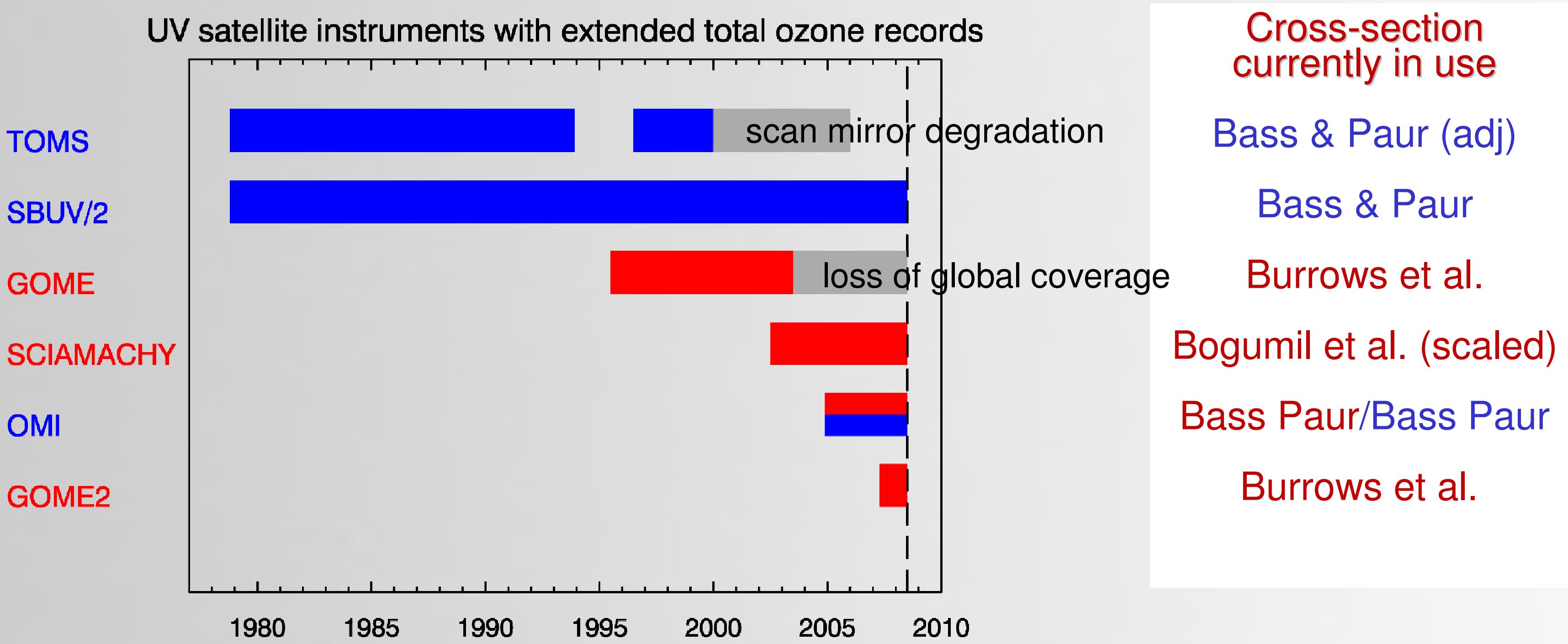
M. Weber, W. Chehade, A. Serdyuchenko, J. P. Burrows
Universität Bremen FB1, Institut für Umweltphysik (iup)

weber@uni-bremen.de http://www.iup.uni-bremen.de/UVSAT

Topics

- DOAS total ozone retrieval from satellites
- Relevant ozone cross-sections
- Diagnostics:
  - ➔ Temperature dependence
  - ➔ direct comparison of cross-section
  - ➔ wavelength shifts & scaling
- Requirements for new laboratory measurements

Past and current (near) global UV TO3 satellite data



- ➔ BUV/Nimbus 4 has been reprocessed (1970-1980), but severe calibration problems
- ➔ TOMS and SBUV TO3 retrievals relies mainly on dicrete wavelengths, e.g. pair/triple retrieval (Dobson like) or optimal estimation
- ➔ GOME/SCIAMACHY/GOME2 use the DOAS technique (differential optical absorption spectroscopy).
- ➔ OMI uses both (OMI-TOMS, OMI-DOAS)

DOAS total ozone retrieval and ozone temperature

Weighting function DOAS

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

Radiation transfer model

Coldewey-Egbers et al., 2005

"Standard" DOAS

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

$$TOZ = (SC_1 + SC_2)/AMF$$

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

Radiation transfer model

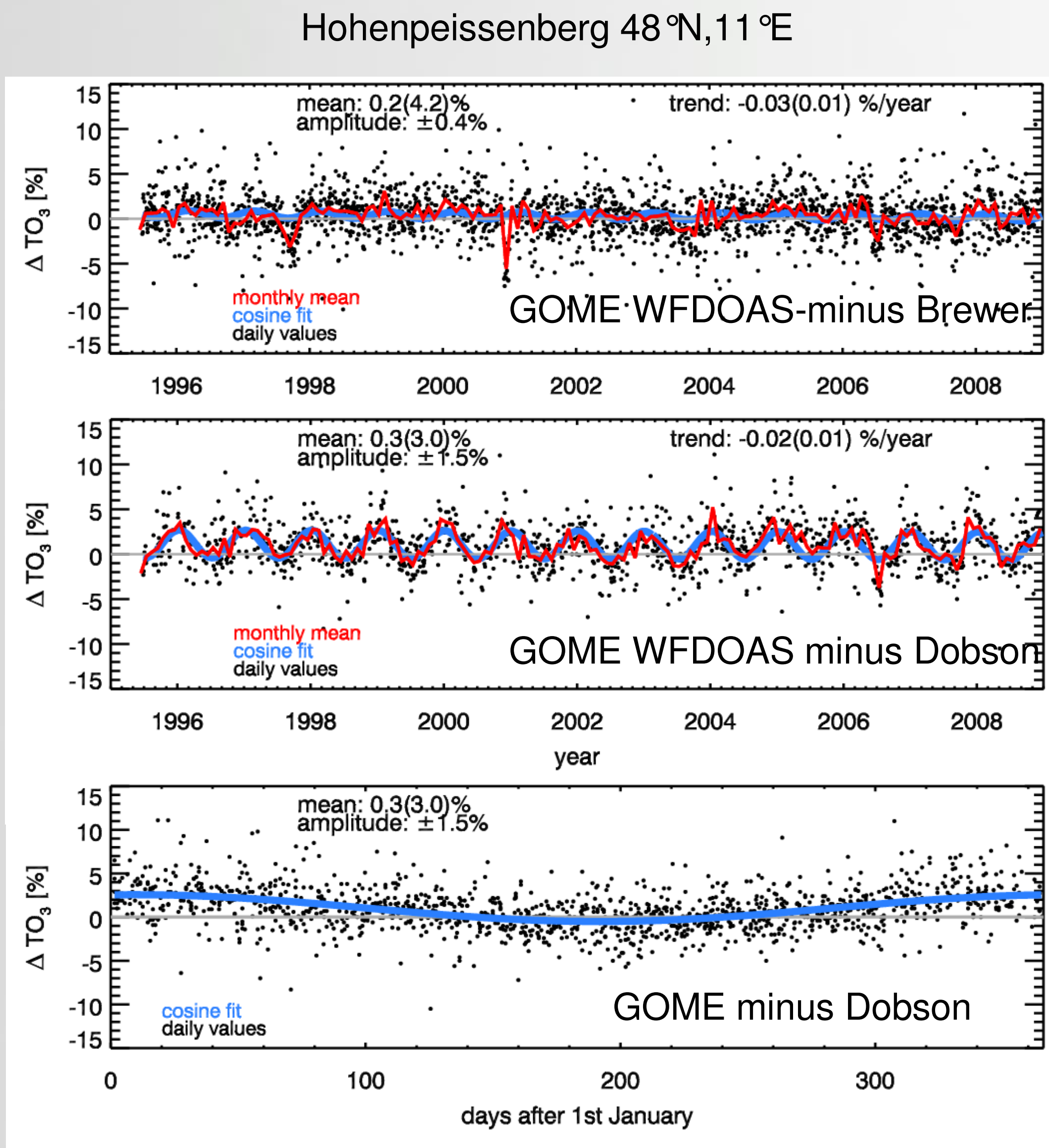
Roozendael et al., 2006

➔ DOAS satellite retrievals

- 325-335 nm
- three methods (all accounting for T-dependence in σ)
  - Weighting function doas (Coldewey-Egbers et al., 2005, Weber et al., 2005)
  - Standard DOAS: ESA operational retrieval (Roozendael et al. 2006)
  - Empirical AMF DOAS (OMI-DOAS): uses ECMWF T-profiles, (Eskes et al., 2005, Vefkind et al., 2006)

Brewer-Dobson comparison at Hohenpeissenberg

- Very good agreement, higher seasonality in the differences with Dobsons
- Error sources:
  - ➔ temperature dependence of cross-section (constant 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)
  - ➔ straylight issue at high SZA (all instruments)



Cross-section data for satellite/ground retrievals

- 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 (Spietz et al.,)
    - T=(203 K), 223 K, 243 K, 273 K, 293 K
    - spectral resolution: 0.29 nm @ 330nm
  - ➔ Bass-Paur (Paur and Bass, 1985)
    - T=203 K, 218 K, 228 K, 243 K, 273 K, 298 K
    - spectral resolution: ~0.1 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 ℃, λ wavelength in nm):

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

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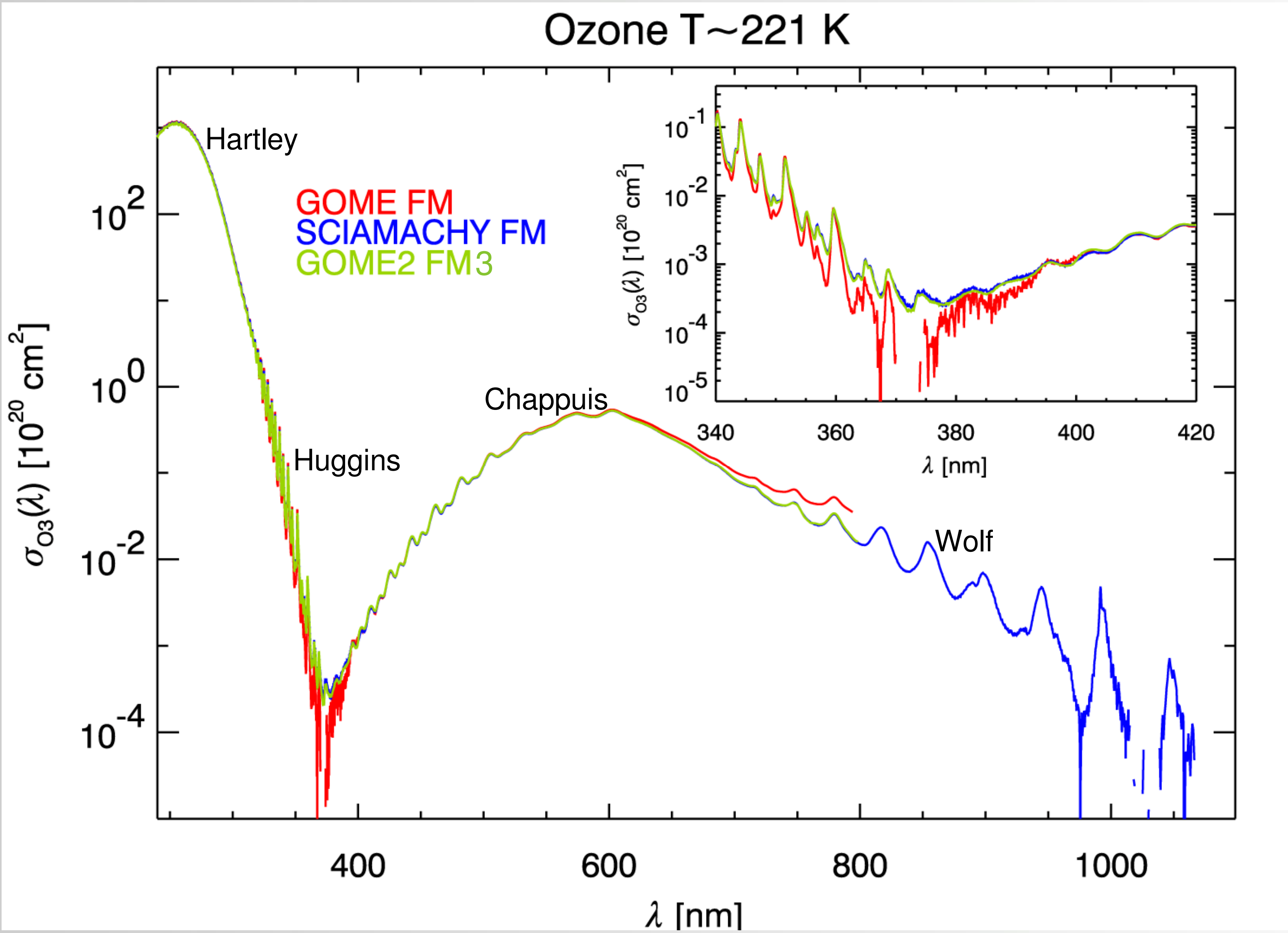
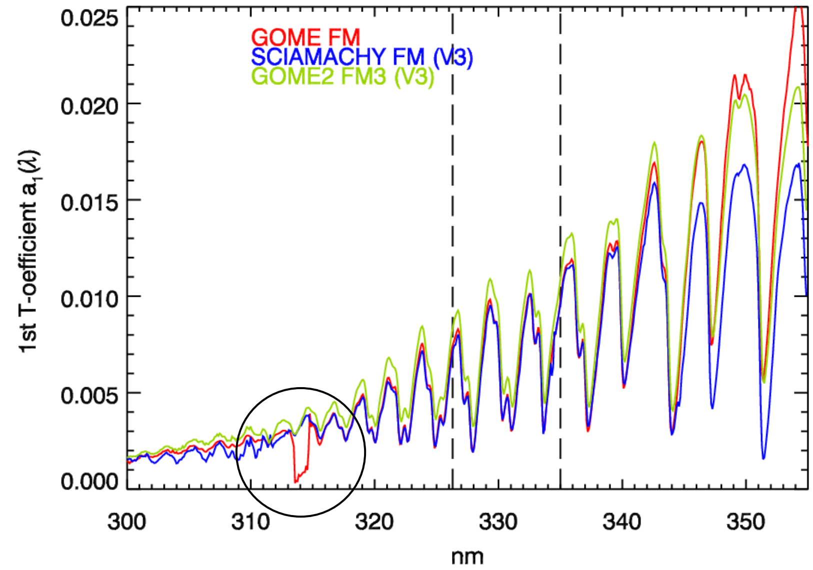
ozone cross-sections from the UV to NIR

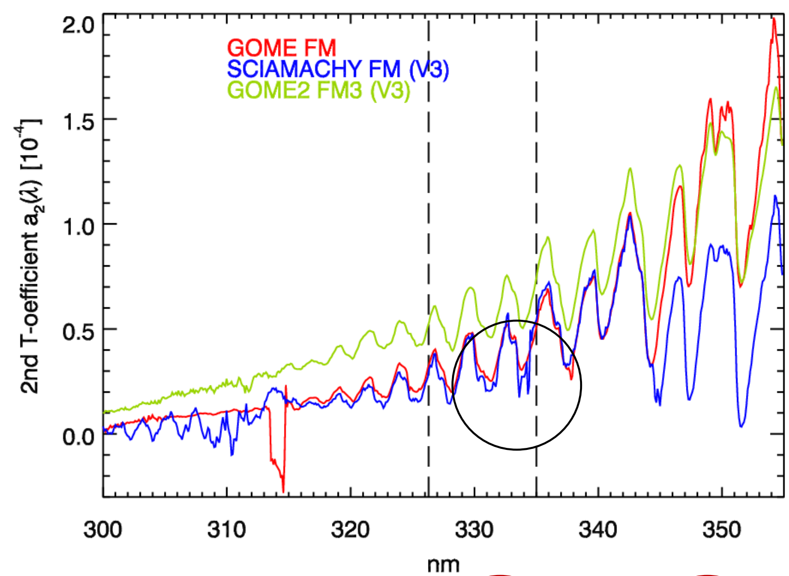


▶Definition of ozone bands

Temperature parameterization

- Problems:
  - ➔ GOME FM: Overlap region between Channel 1 and 2 (~315 nm)
  - ➔ SCIAMACHY FM: overlap region (Ch. 1&2), ~334 nm
  - ➔ GOME2 FM3: different temperature dependence

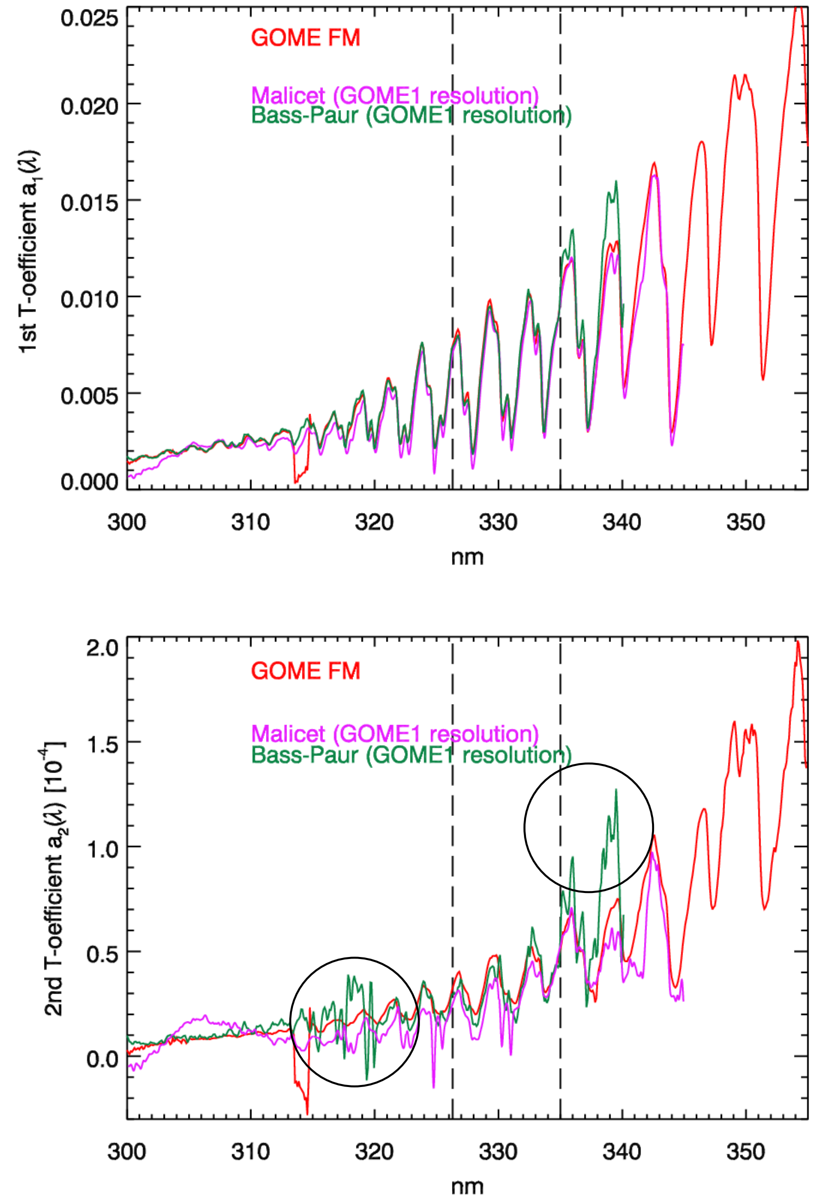




$$\sigma(\lambda, t) = a_0(\lambda)\left[1 + a_1(\lambda)t + a_2(\lambda)t^2\right]$$

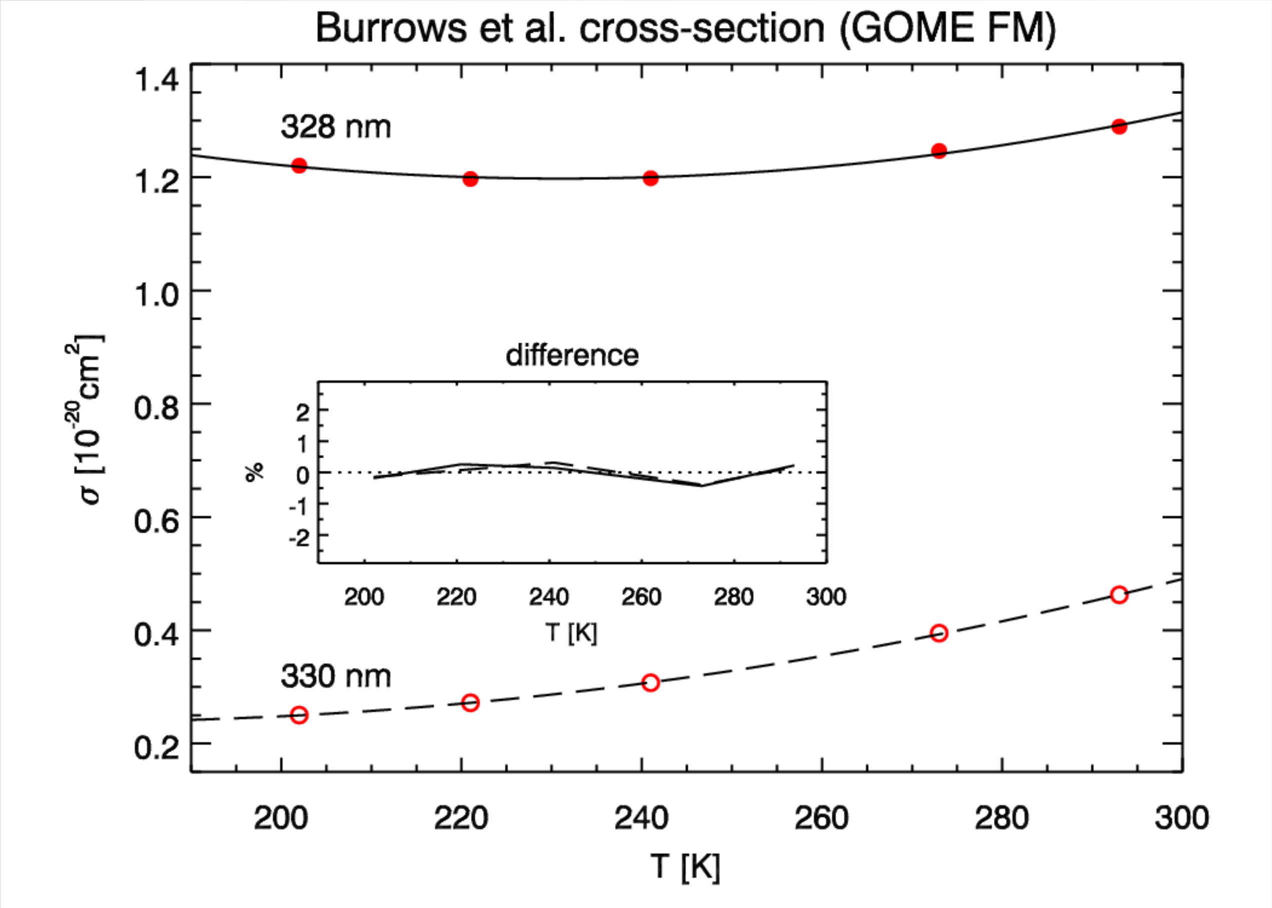
Temperature parameterization II

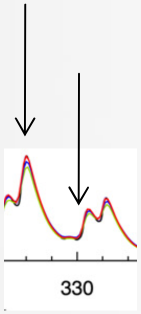
- Problems with other data:
  - ➔ Bass-Paur: noisier, particularly 315-320 nm
  - ➔ Above 335 nm, Bass-Paur extended with Vigroux(?)
  - ➔ Malicet: fairly consistent, slightly different temperature behaviour (second coefficient sometimes negative)



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

Consistency of cross-sections: Bass-Paur parameterisation I

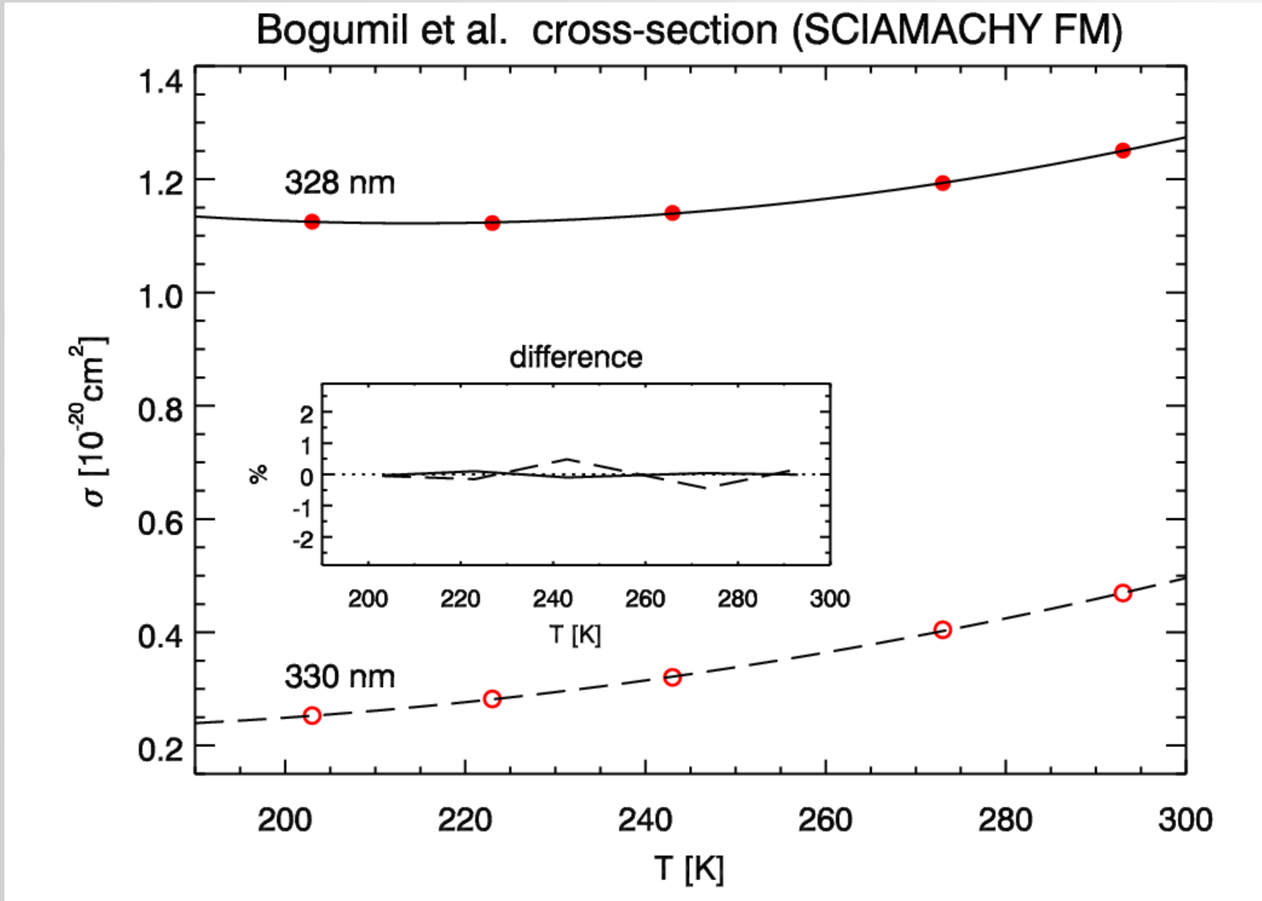


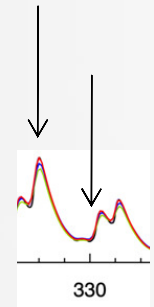


$$\sigma(\lambda, t) = a_0(\lambda)\left[1 + a_1(\lambda)t + a_2(\lambda)t^2\right]$$

- ▶ GOME FM:
  - ➔ Differences at individual temperatures below 0.5%

Consistency of cross-sections: Bass-Paur parameterisation II



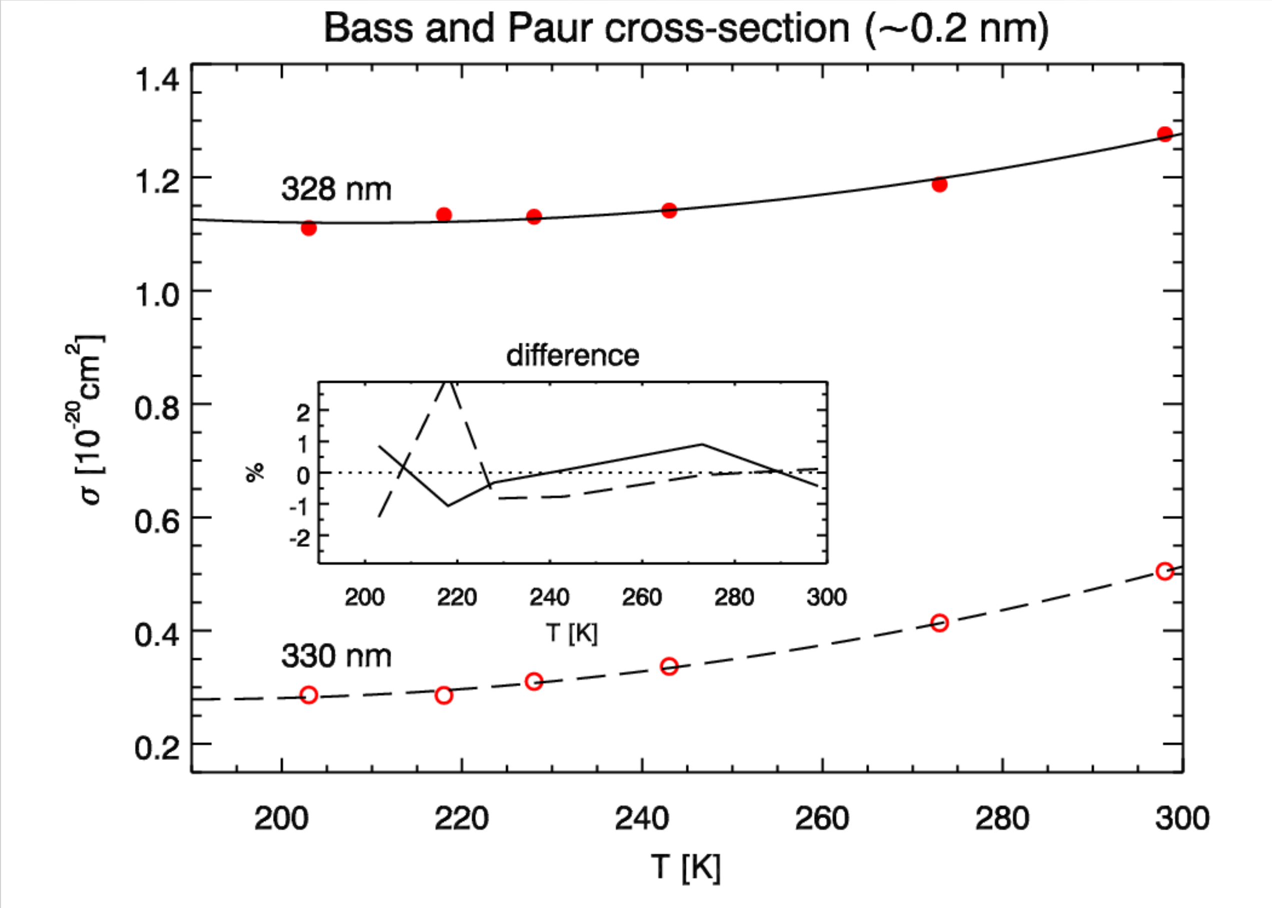


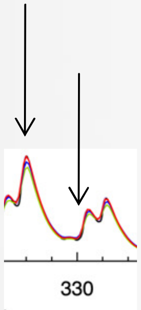
$$\sigma(\lambda,t) = a_0(\lambda)\left[1 + a_1(\lambda)t + a_2(\lambda)t^2\right]$$

▶ SCIA FM:

- ➔ Differences at individual temperatures below 0.5%
- ➔ Changes from GOME FM to SCIA FM larger near absorption maximum (328 nm)

Consistency of cross-sections: Bass-Paur parameterisation III

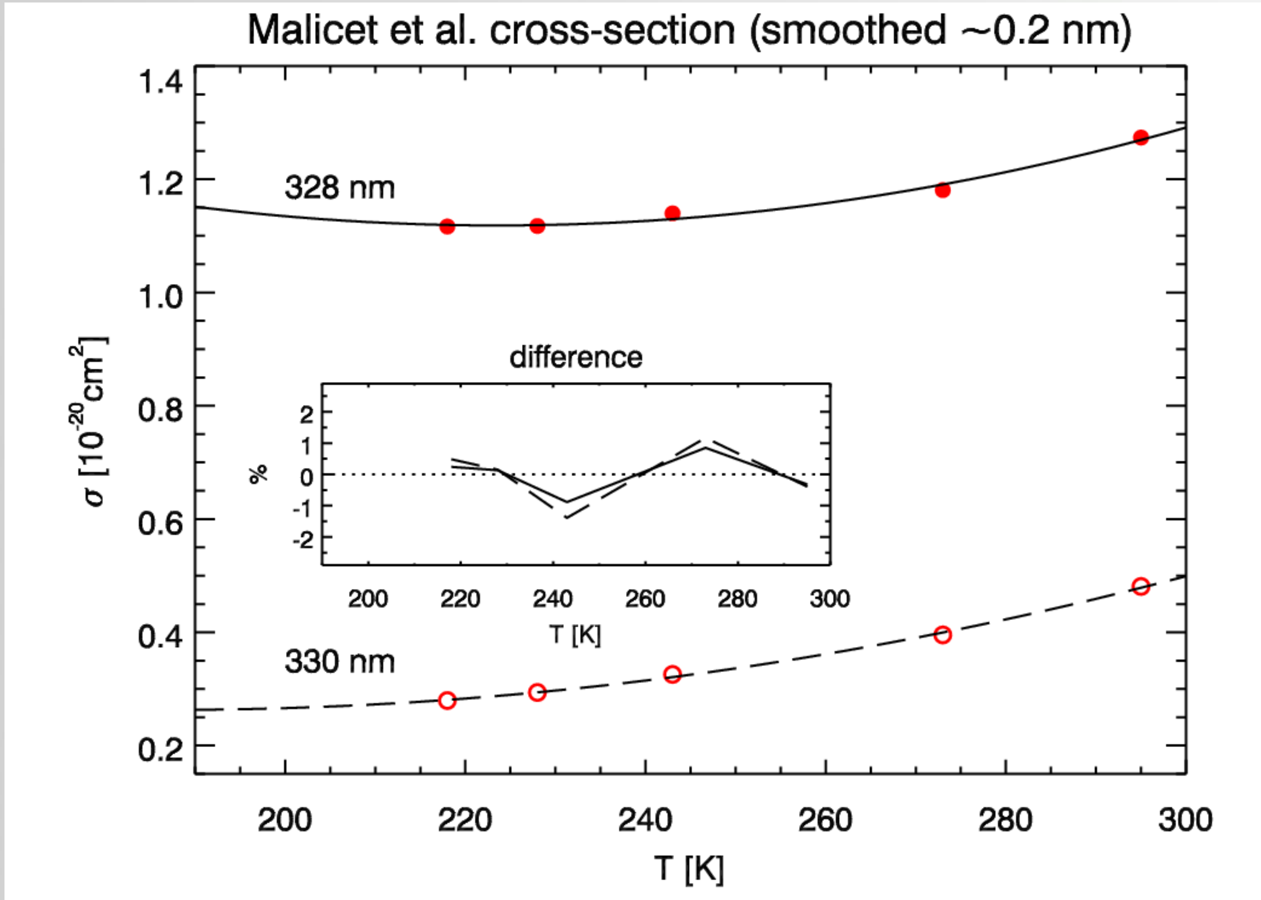


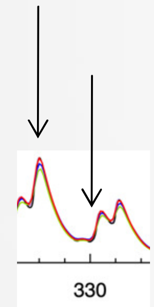


$$\sigma(\lambda, t) = a_0(\lambda)\left[1 + a_1(\lambda)t + a_2(\lambda)t^2\right]$$

- Bass-Paur:
  - ➔ Differences at individual temperatures close to 3% (218 K)!

Consistency of cross-sections: Bass-Paur parameterisation III





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

- Bass-Paur:
  - ➔ Differences at individual temperatures close to 3% (218 K)!
- Malicet et al:
  - ➔ different behaviour at low T: T<218 K

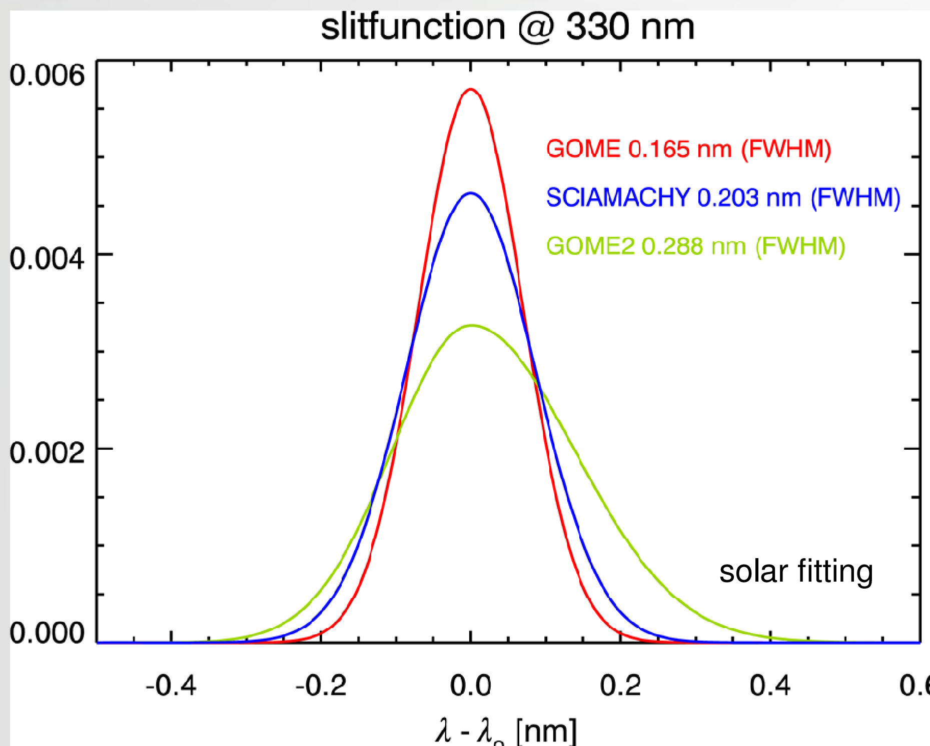
Slit function fit

- (Transfer) 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)
    - Gaussian (sym)
    - Doppel-Voigt (assym)
  - ➔ Polynomial: *Pol(λ)*

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



Cross-section issues in satellite DOAS I

Cross-sections	T[K]	Shift [nm]	FWHM [nm]	solar FWHM [nm]	Scaling [-]	Scaling wrt GOME1
Burrows et al. 1999 GOME FM	225 240	+0.017(2) +0.017(2)	0.158(5) 0.159(6)	0.165(8)	1.027(2) 1.023(2)	- -
Bogumil et al. 2003 SCIAMACHY FM	225 240	+0.008(2) +0.009(2)	0.222(6) 0.219(6)	0.202(13)	0.970(3) 0.973(3)	0.944 0.951 -5%
Spietz et al. GOME2 FM3	225 240	-0.047(2) -0.046(2)	-	0.286(27)	0.950(7) 0.938(6)	0.925 0.917 -8%

- Slitfunction fits w.r.t. Malicet cross-sections: 326.6-334.5 nm
  - ➔ Shifts minimising fit residuals in WFDOAS agree with shifts from cross-section comparisons (good wavelength calibration for Malicet et al.)
  - ➔ SCIAMACHY FM requiring a scaling of +5% wrt to GOME1,
- GOME2-FM3 under investigation (large shift and scaling)
- Total ozone change is -6DU/0.01nm shift (or -2%/0.01 nm) !!!

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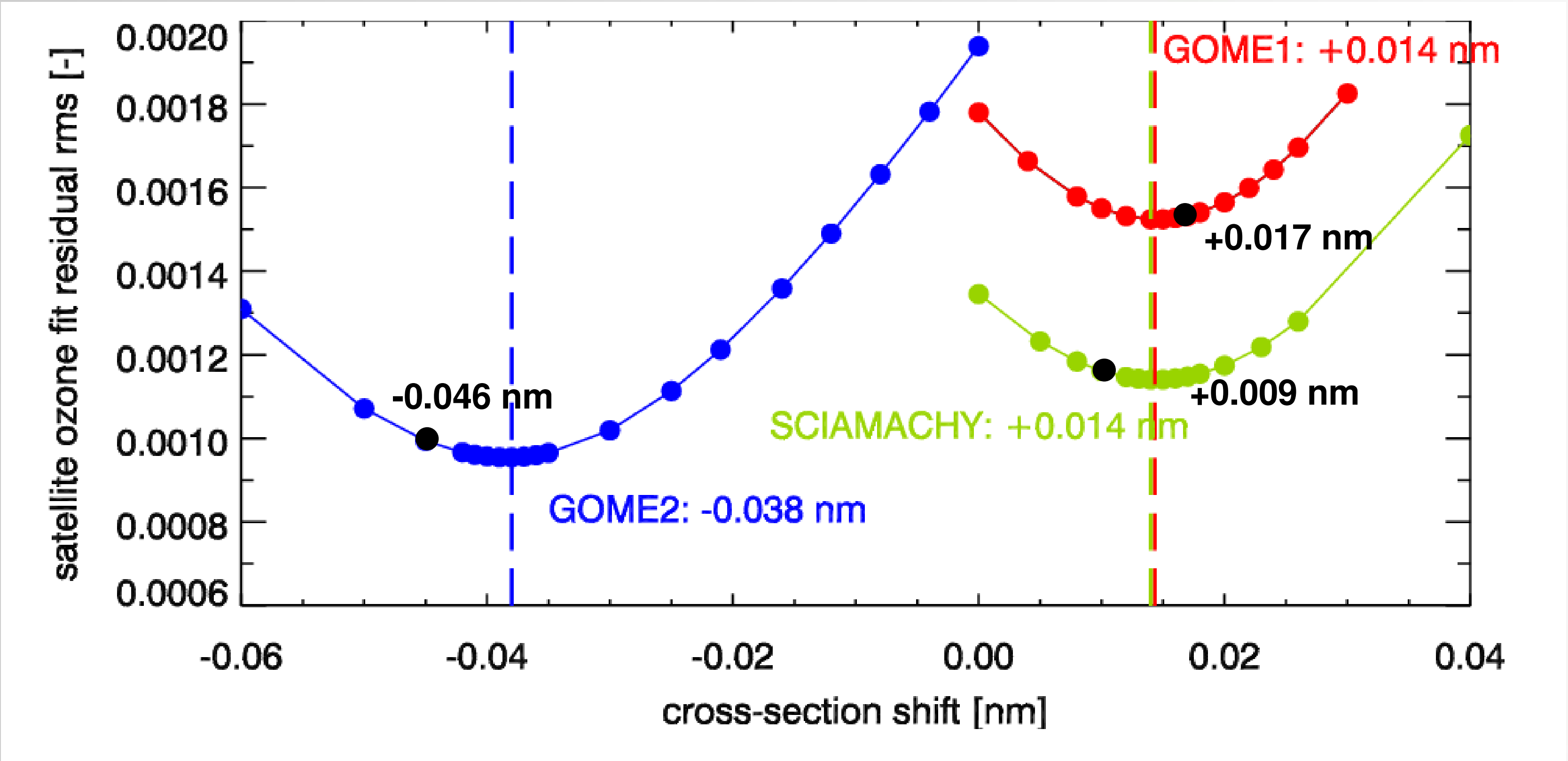
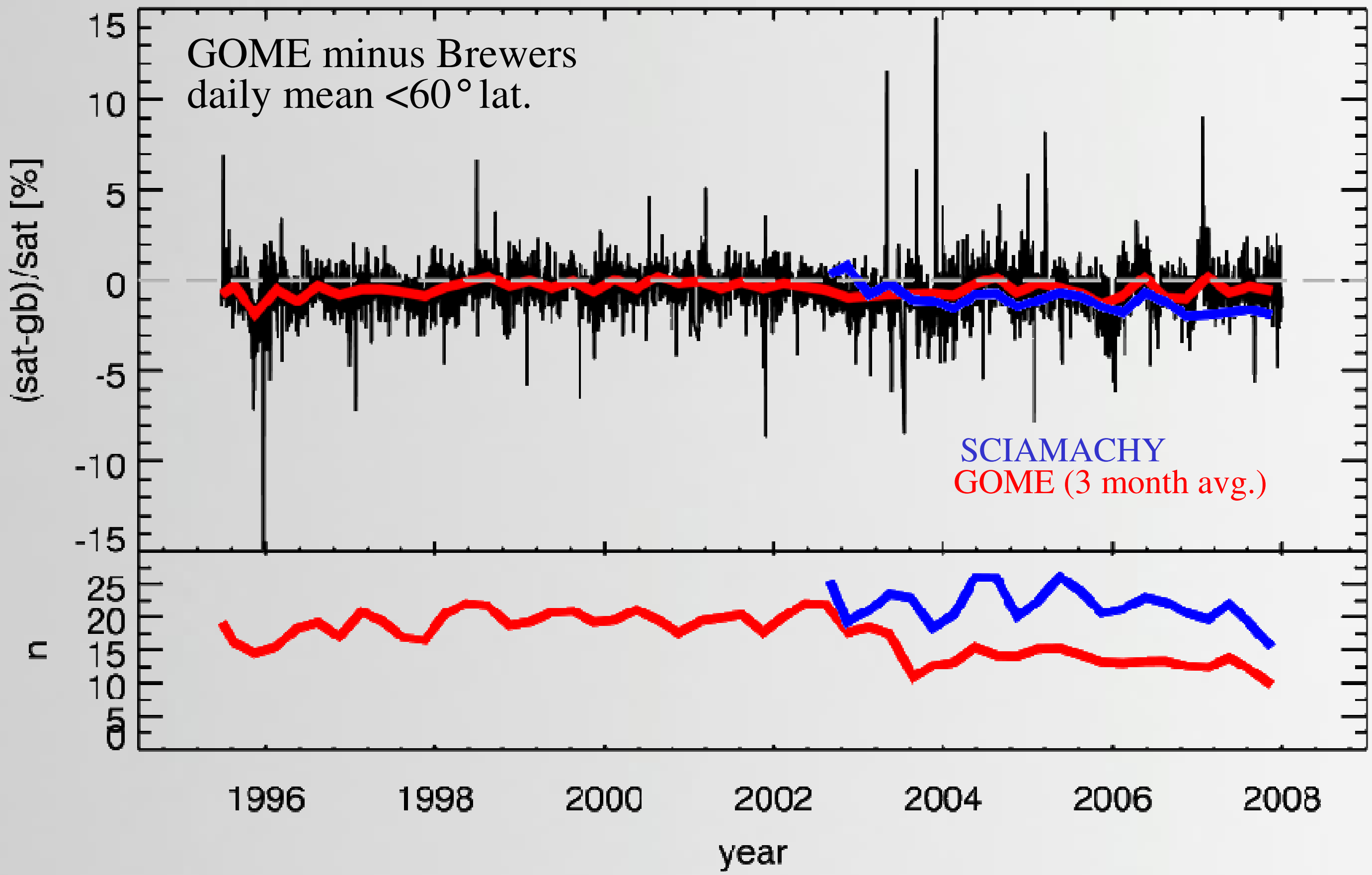
Cross-section issues in satellite DOAS II



Ozone fit residual RMS for GOME1, SCIAMACHY, and GOME2 as a function of cross-section shifts. Black dots indicate optimum shifts from direct comparisons between cross-sections with respect to a shift of 0.017nm in GOME1 as used in WFDOAS V1.

- Cross-section shifts are nearly consistent with minimum fit residual RMS requirements and wavelength calibration of Kitt Peak solar atlas (“Fraunhofer fitting”)
- Fit residuals are lowest with GOME 2

Satellite-Brewer difference time series



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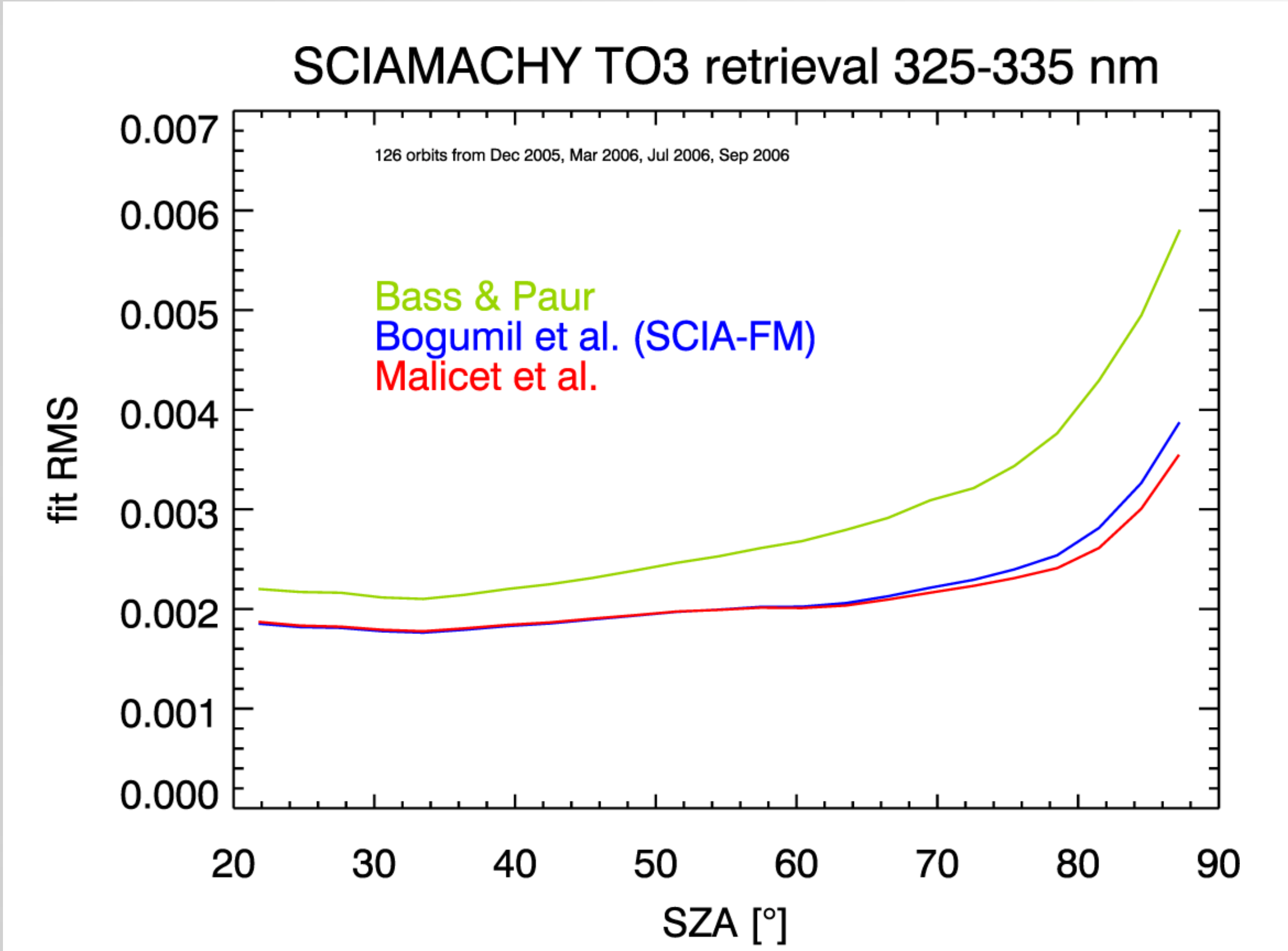
- Using scaled SCIAMACHY FM good consistency with GOME
- Comparison between satellites and with Brewers show a downward trend in SCIAMACHY of about -0.4%/year (algorithm independent, level-1 calibration issue, see also Lerot et al. 2009)

Use of various cross-sections in WFDOAS retrievals



- With optimum shifts and slit function convolution retrievals show similar fit rms for Malicet and GOME/SCIA/GOME2 FM, Malicet slightly better at high SZA
- Bass Paur leads to higher fit residuals

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 (see next talk by Anna Serdyuchenko)
  - ➔ Reanalysis of GOME, SCIA, and GOME2 x-section data

Requirements on UV/Vis O3 x-section measurements

- Important wavelength regions:
  - ➔ 240-330 nm: nadir profile retrieval
    - Absolute x-section
  - ➔ 305-335 nm: nadir column retrieval
    - Temperature dependence, wavelength calibration
  - ➔ 335-380 nm: auxiliary retrieval for OClO, BrO, O4, NO2, H2CO, glyoxal
  - ➔ 240-600 nm: Limb scatter UV/VIS (Hartley-Huggins-Chappuis, 10-65 km altitude)
- Verification by retrieval studies
  - ➔ Minimisation of fit residuals using solar reference (Fraunhofer fitting) and proper wavelength shifts in x-section
  - ➔ Verification of retrieved ozone temperatures with meteorological analysis and atmospheric data