Impact of Serdyuchenko et al. cross-section on DOAS satellite retrievals (325-335 nm)

A contribution to WMO-GAW/ IO3C
IGACO-O3 Absorption Cross-Sections of Ozone Activity (ACSO)

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New/updated cross-section data at IUP

- New broadband high spectral resolution UV/VIS/NIR ozone cross-section (Serdyuchenko et al.)
  - Serdyuchenko et al., Gorshelev et al., submitted to AMTD
- Updated SCIAMACHY FM (Bogumil et al.) and revised GOME-2 FM3 (Metop A) cross-sections
  - Chehade et al., AMTD, 2012 & 2013

DOAS total ozone retrieval and ozone temperature

Weighting function DOAS

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

Coldewey-Egbers et al., 2005

Radiation transfer model

retrieved total ozone

retrieved ozone temperature

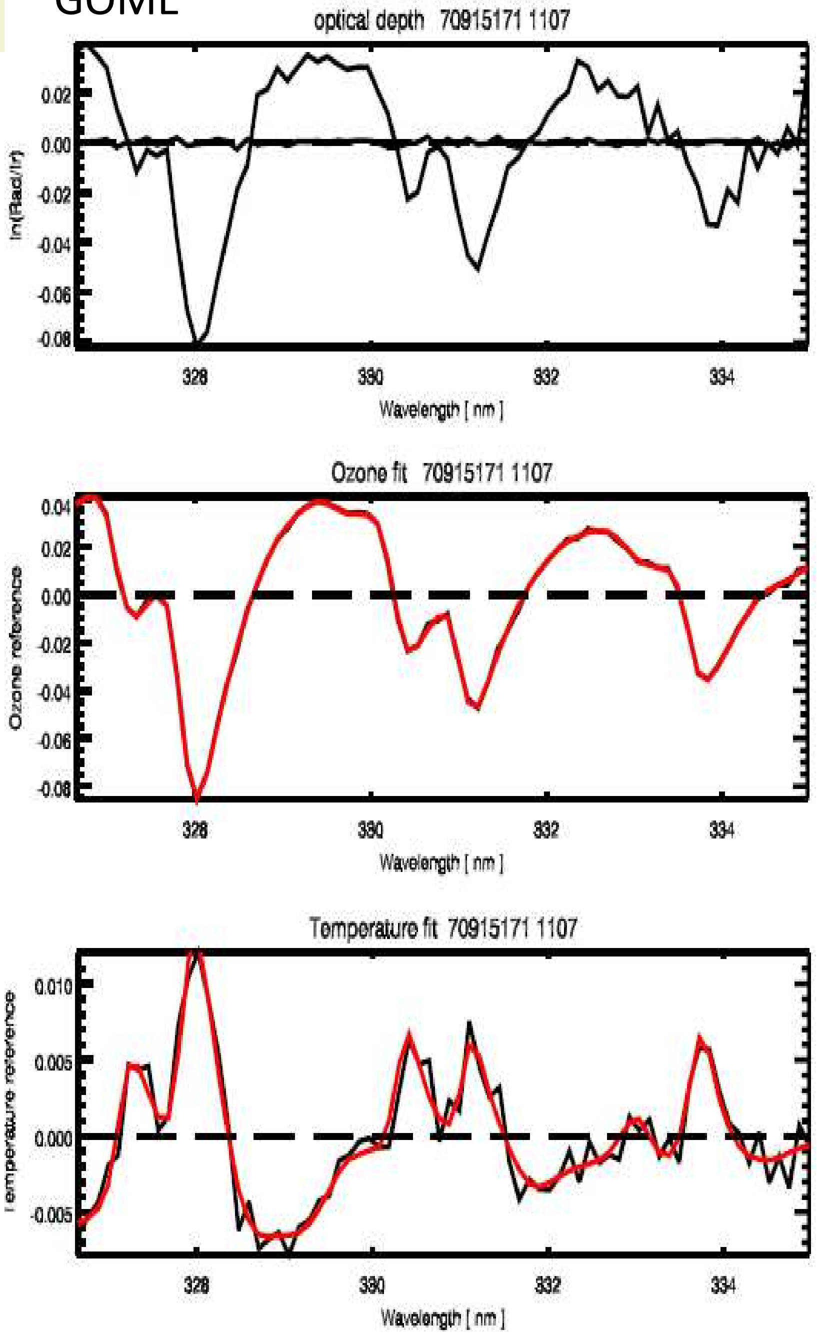
The retrieved scalar temperature correction effectively accounts for the dependence of the observed ozone absorption on stratospheric temperature.

- DOAS satellite retrievals (OMI, GOMEs, SCIAMACHY)
  - 325-335 nm (WFDOAS: 326.6-334.5 nm)
- U Bremen retrieval: Weighting function DOAS *(Coldewey-Egbers et al., 2005, Weber et al., 2005, Lee et al., 2008)*
  - Weighting functions: the relative radiance change due to a vertical profile change assuming an altitude independent scaling factor
  - scalar temperature shift in the a-priori temperature profile
  - effective ozone temperature T_{O3}

- Both total ozone and temperature depend on ozone cross-section choice

Ozone and temperature terms in WFDOAS equation

GOME

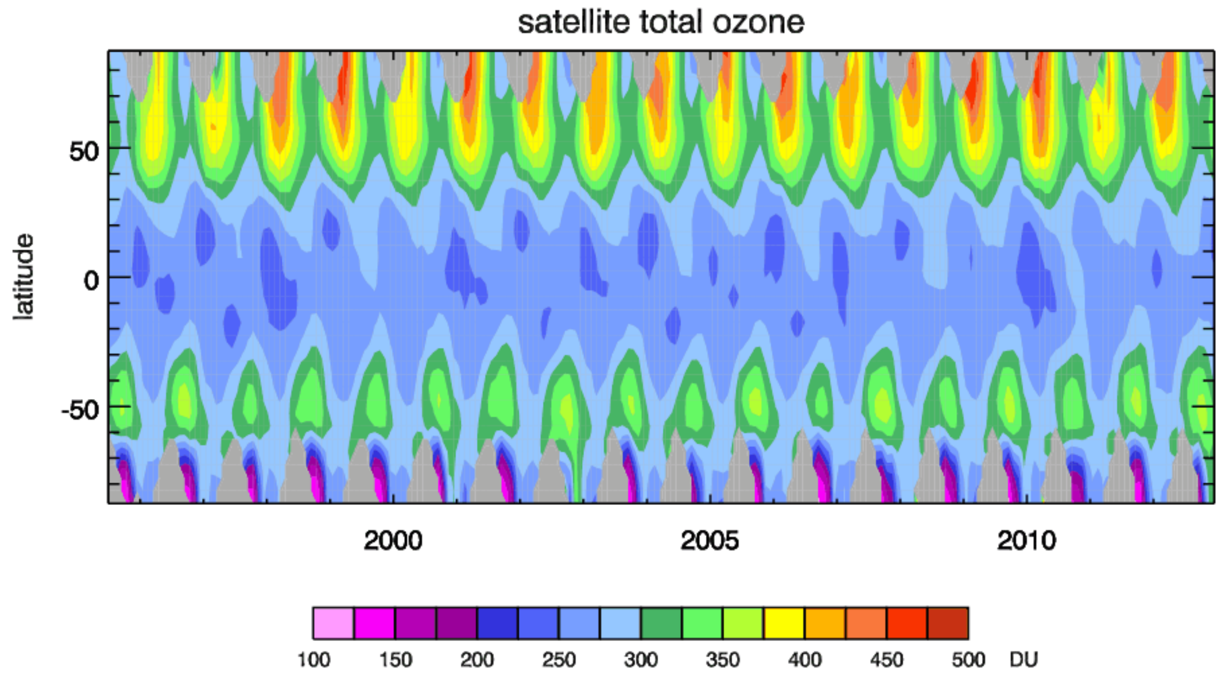


$$\ln \frac{I_{obs}}{F_{obs}} = \ln\left(\frac{I}{F}\right)_{mod} + \frac{d\ln(I/F)}{d\mathrm{TOZ}}\Big|_{mod} (\mathrm{TOZ}_{fit} - \mathrm{TOZ}_{clim}) + \frac{d\ln(I/F)}{d\mathrm{T}}\Big|_{mod} (\mathrm{T}_{fit} - \mathrm{T}_{clim}) + \ldots + \mathrm{Pol}$$

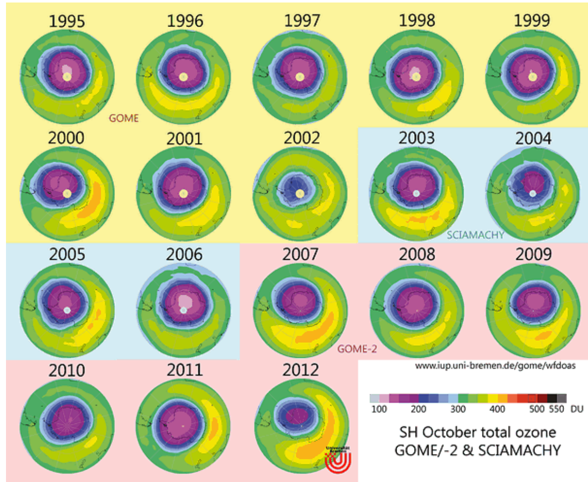
- Fit residual in GOME orbit 70915171.
- The GOME observed differential optical depth and fit residual
- magnitude of the various terms in the WFDOAS equation.
- Red lines show the modeled values and the fit residual has been added to each term (black) to visualize the relative magnitude of the measurement noise
  - 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

WFDOAS total ozone data sets & cross-section used



merged WFDOAS data record
(Weber et al. 2011, 2012)



- WFDOAS applied to GOME (1995-2011), SCIAMACHY (2002-2012), and GOME-2 (since 2006)
  - GOME1/ERS : Burrows et al. 1999 (GOME FM), shift: +0.017 nm
  - SCIAMACHY/ENVISAT: Bogumil et al., 2003 (SCIA FM), scaled 5.3%, shift: +0.008 nm
  - GOME2/METOP A: Burrows et al., 1999, convolved, shift: +0.017nm
- agreement to within 1% with WOUDC brewer and dobsons
- Nevertheless: use of a single cross-section data for all instruments are needed to better understand calibration differences between instruments

Direct comparisons of ozone cross-sections

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

Serdyuchenko et al.

Scaling factor (differential)

BMD or Bass Paur (ACSO)

shift

slit function, here $\delta(\lambda-\lambda')$ (only needed for comparisons with low spectral resolution cross-section)

cubic polynomial (differential fitting)

- Differential scaling between high resolution ozone cross-sections in DOAS window (fit parameters: scaling factor, wavelength shift, and polynomial)

Direct comparison in DOAS window (325-335 nm)

Cross-sections	T [K]	Scaling factors [-]	Shift [nm]
BMD	218 227 238	1.0128(10) 1.0145(09) 1.0142(12)	- - -
Bass Paur (ACSO)	218 227 238	1.0096(31) 1.0115(29) 1.0119(29)	0.0307(8) 0.0292(7) 0.0278(7)

**scaling and shifts to match Serdyuchenko et al.*

*** x-sections as polynomial quadratic in T*

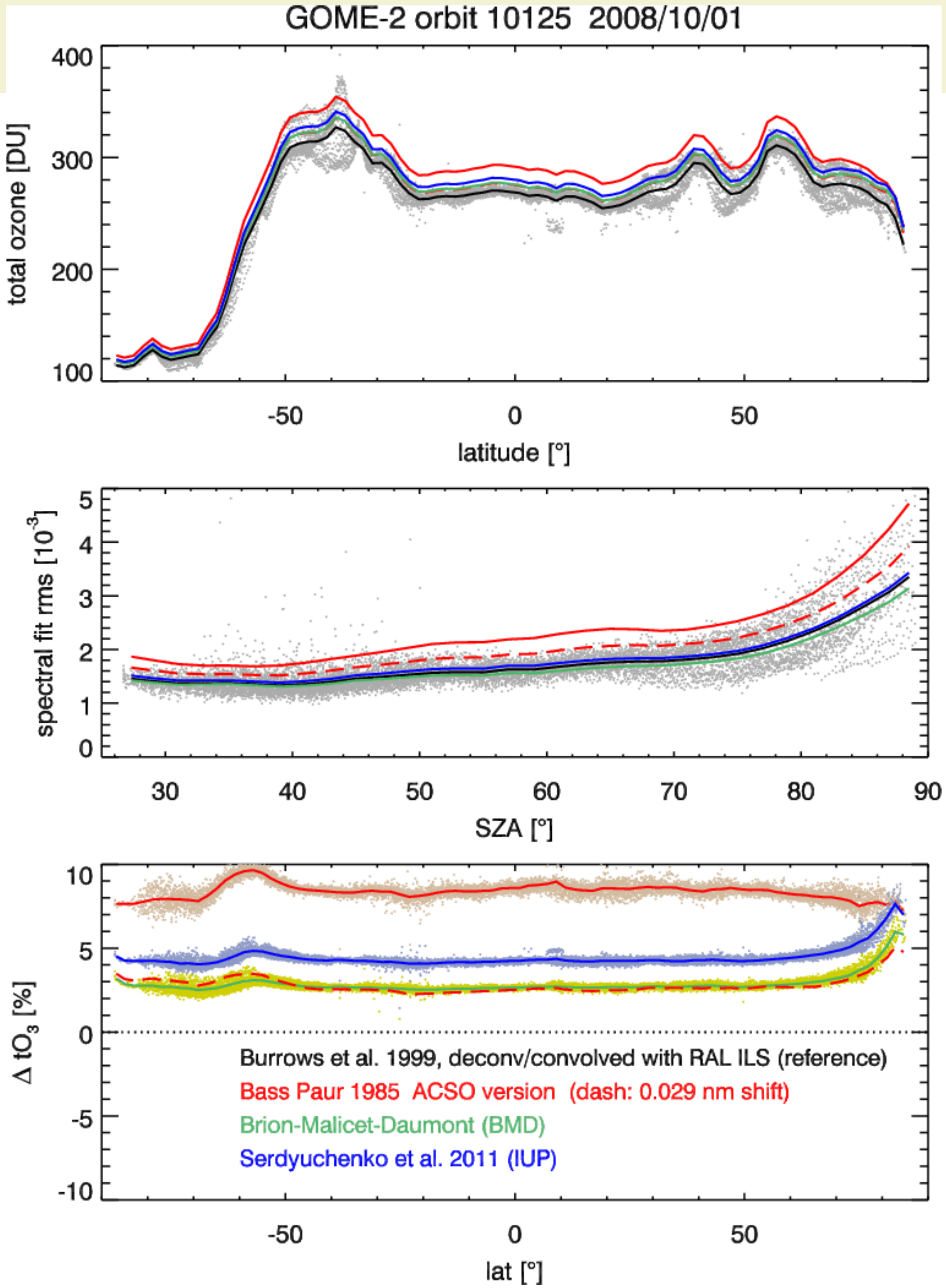
- agreement with BP and BMD (<1.4%) within experimental uncertainty of laboratory measurements (2-3%)

- BMD has to be scaled by ~1.4% (should lead to 1.4% lower total ozone than Serdyuchenko in DOAS retrieval)
- BP (with 0.029 nm shift) has to be scaled 1.1% (should lead to 1.1% lower ozone than Serdyuchenko et al.)
- significant wavelength shifts of Bass Paur data (note: ozone sensitivity is about -6 DU per 0.01 nm shift at GOME/SCIA spectral resolution!)

Note: Bass Paur (ACSO) are quadratic coefficients excluding 218 K data

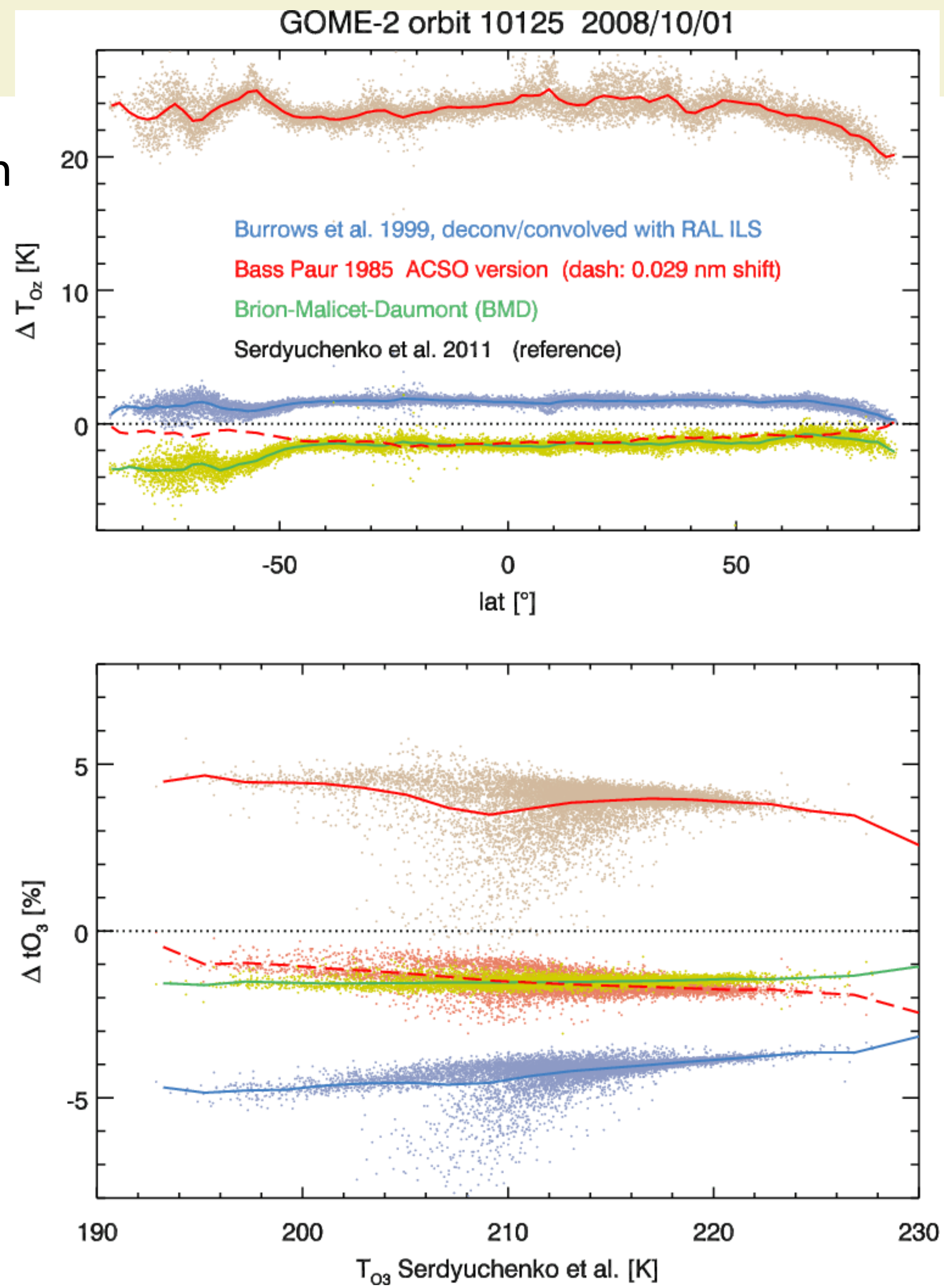
Retrieval impact: GOME-2

- Spectral fit residuals lowest with BMD and Serdyuchenko
- Bass Paur noisier
- Ozone:
  - Serdyuchenko ~1.5% higher than BMD and Bass Paur shifted by 0.029 nm(!)
  - BMD and Bass Paur shifted by 0.029 nm(!) agree within 1%
  - Bass Paur without wavelength shift show larger deviations
- Ozone results are as expected from the direct comparisons between cross-sections (incl. Burrows et al.)



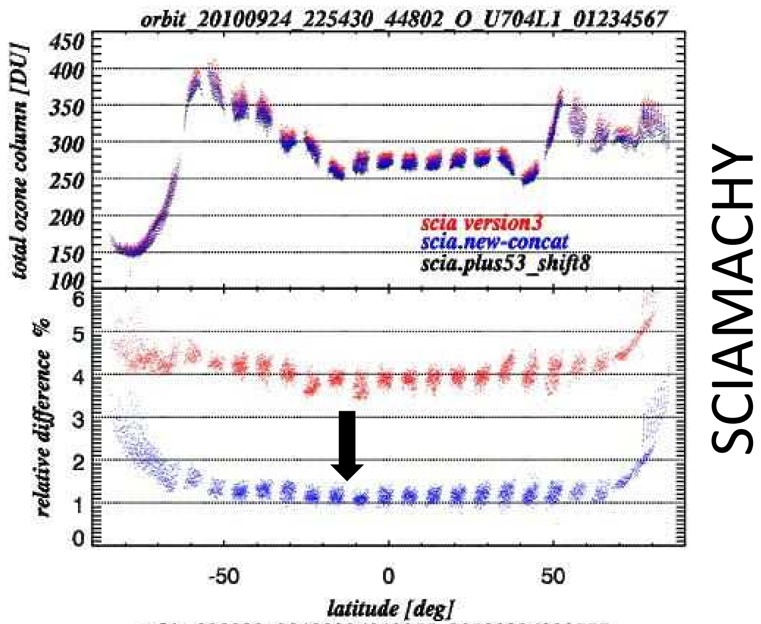
Temperature dependence

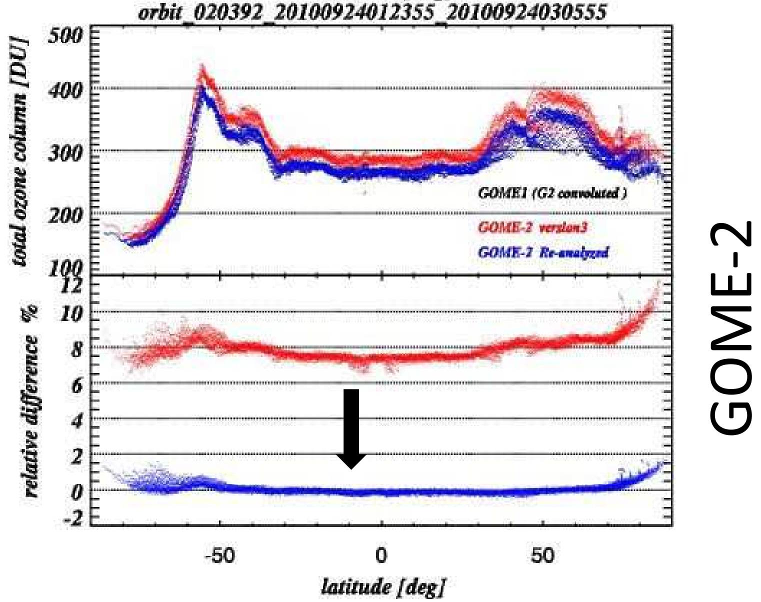
- Without shifts BP leads to +25 K bias in retrieved ozone temperatures (within 2K with shifts)
- BMD, Burrows et al. and shifted BP ozone temperature are within 2K wrt Serdyuchenko et al.
- Low bias in ozone and T_{O3} retrieved with BMD in Antarctic ozone hole condition (cold bias)
- Sensitivities of ozone differences wrt T_{O3} varies and are on the order of -1% to 1% DU per 20 K change between BMD, BP, and Serdyuchenko et al. cross-sections



Impact from revised satellite FM cross-sections

- WFDOAS retrieval tests of new satellite FM updates using one SCIA and one GOME-2 orbit
  - optimal shift of x-section by minimising fit residuals
    - » SCIA FM: +0.017 nm
    - » GOME-2 FM: -0.038 nm
- agreement now to within 1% with standard WFDOAS retrieval and GOME/ERS
- SCIAMACHY's and GOME -2 total ozone column retrievals with different cross section data
  - Scia.plus53.shift8 is the SCIAMACHY FM data (Bogumil et al., 2003) with a differential scaling of +5.3% and shift of 0.08nm from a direct comparison to GOME FM cross-sections (Weber et al., 2011) as used in the current standard retrieval.
- The lower sub-panels show the difference to the retrieved ozone using scia.plus53.shift8 cross-sections and GOME 1 (G2-convolved).





Chehade et al., 2012, 2013

Conclusion

- in the classic DOAS window (325-335 nm) Serdyuchenko et al. deliver total ozone 1.0-1.5% higher than BMD and (shifted!) BP
- new Serdyuchenko et al. ozone cross-sections are available
  - broad spectral coverage (UV/vis/NIR), many T's (11), high spectral resolution (0.02-0.03 nm)
  - see talk by Serdyuchenko et al.
- satellite FM cross-section (SCIA FM=Bogumil et al., GOME-2 FM3) at medium spectral resolution (~0.2-0.4 nm) have been significantly improved by reanalysis
  - do we need satellite FM cross-section? Yes, they are useful for diagnosing satellite instrument performance (spectral resolution, SNR, etc.)
- cross-section data available from:

  http://www.iup.uni-bremen.de/UVSAT_material/data/xsections/

Recommendations?

- DOAS window: all high resolution cross-sections (BMD, BP w/ shift, Serdyuchenko) deliver similar results (within 1.5%)
- But:
  - BP is noisier
  - BMD is somewhat less reliable at very cold temperature (lowest T is 218 K)
  - Serdyuchenko has variable SNR, very similar to BMD in DOAS window, a bit noiser at shorter wavelengths
- Which is best really depends on the wavelenght ranges used and may be retrieval dependent (differential vs absolute fitting)