Total ozone measurements with Phaethon at Izaña including characterizations/calibrations and uncertainty estimations

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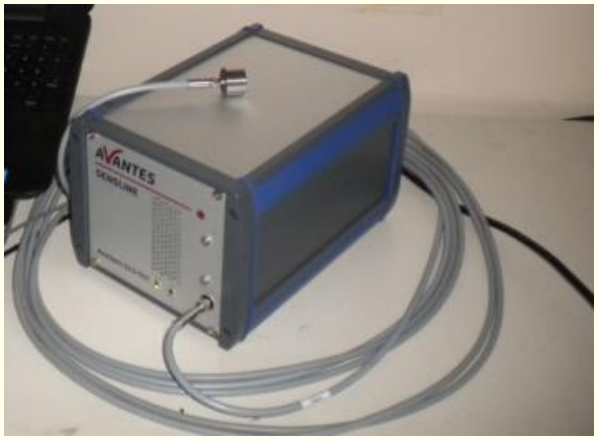
Layout

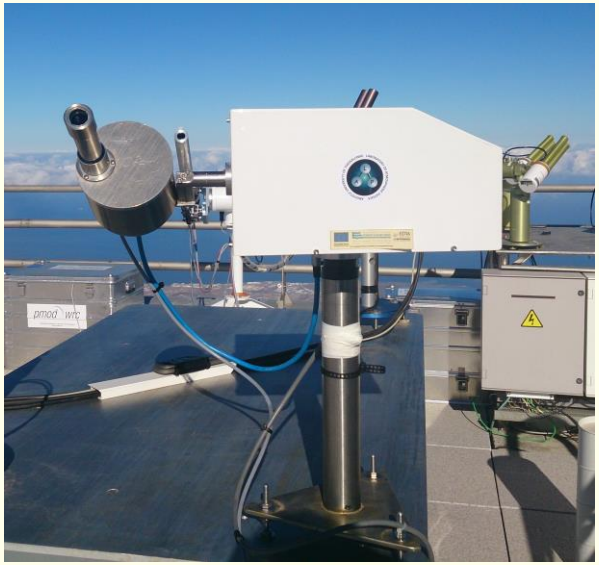
- Brief introduction to DOAS-based retrieval of TOC by Phaethon
- Langley results from Izaña campaign in September 2016
- Comparisons with Brewer TOC data in Izaña and Thessaloniki
- Estimation of data uncertainties

The Phaethon mini-DOAS system

- Spectrometer
  - Cooled miniature CCD spectrograph AvaSpec-ULS2048LTEC
  - Operating temperature: 5 °C
  - Spectral range: 300 - 452 nm
  - Spectral resolution: ~0.25 nm

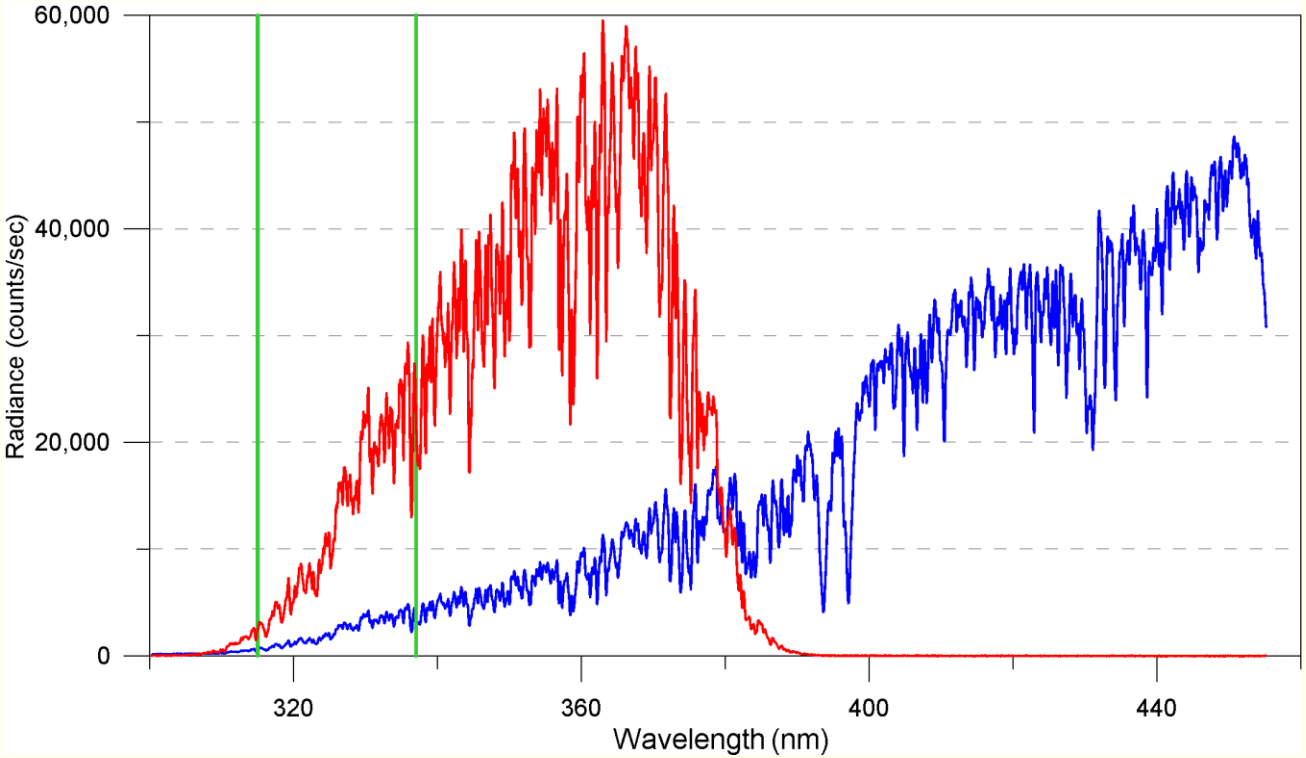


- Entrance Optics for total ozone measurements
  - Direct solar irradiance port with diffuser and ND filter
  - Far field stray light suppression: 475 nm short-pass filter
  - Spectral range modification: UV enhanced (300-370 nm)
  - Filed of View (~1°)



Range of TOC retrieval 315 - 337 nm

- TOC is retrieved from both regular and UV-enhanced spectra
- UV-enhanced range:
  - increases intensity by a factor of 5
  - reduces far-field stray-light effect from longer wavelengths
  - reduces DOAS retrieval error



Langley determination of SCD_{REF}

- SCD_{REF}: slant column ozone of the reference spectrum used in DOAS

- DOAS analysis provides the differential slant column density (*dSCD*) of ozone between the analyzed and the reference spectrum:

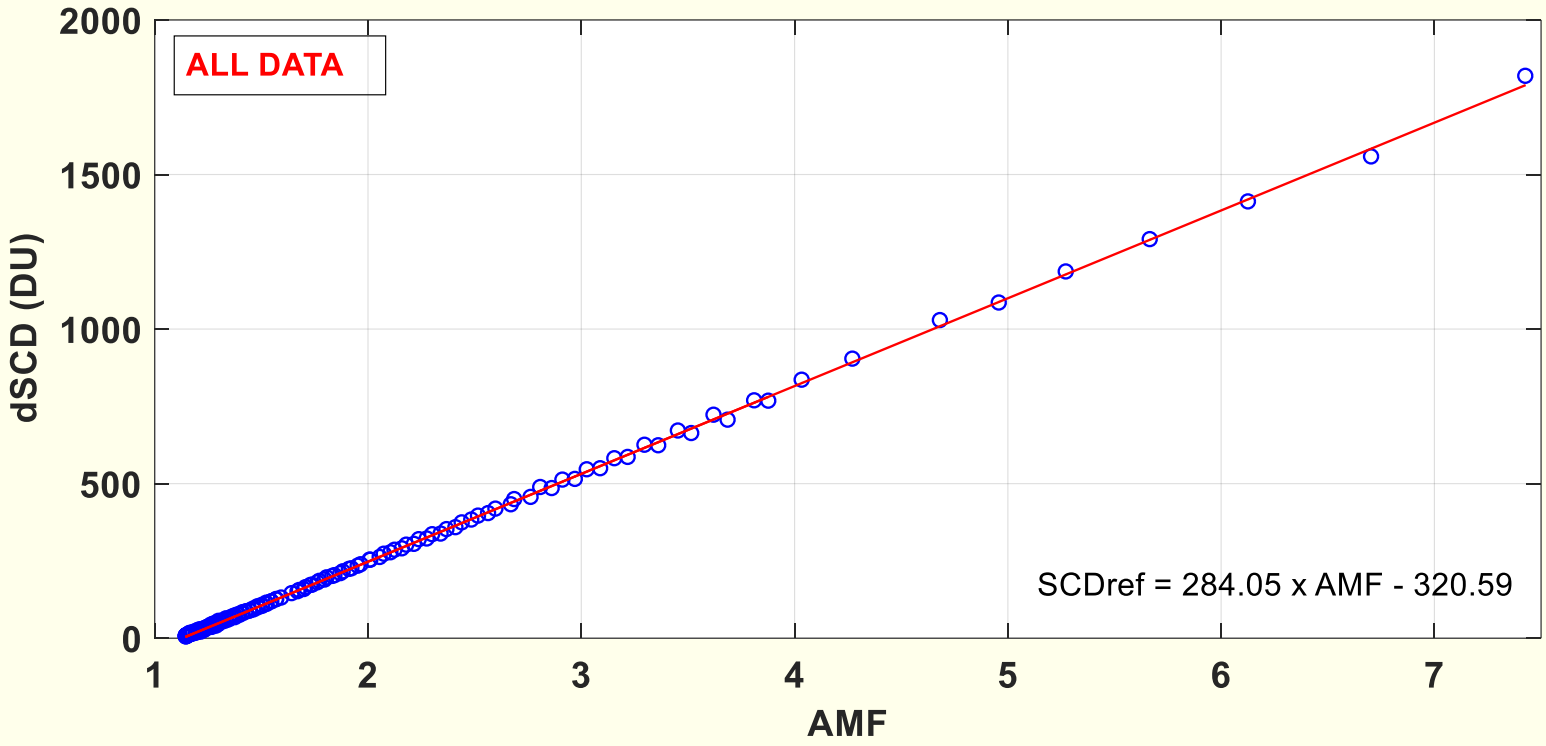
$$dSCD_i = SCD_i - SCD_{REF} = TOC_i \cdot AMF_i - SCD_{REF}$$

- SCD_{REF} is derived from Langley extrapolation of *dSCD* vs *AMF*

- Langley plots were derived from data of the Izaña ATMOZ campaign (14-27 September 2016)

- **This dataset can be used to derive the SCD_{REF} of any spectrum recorded by the same spectrometer**

Phaethon Langley plot - Izaña



Removal of outlier points

- Based on work of Kiedron and Michalsky 2016 (AMT)
- by “eye and mind”
- least-squares fitting (LSF) of *dSCD* with respect to *AMF* with sequential removal of outliers

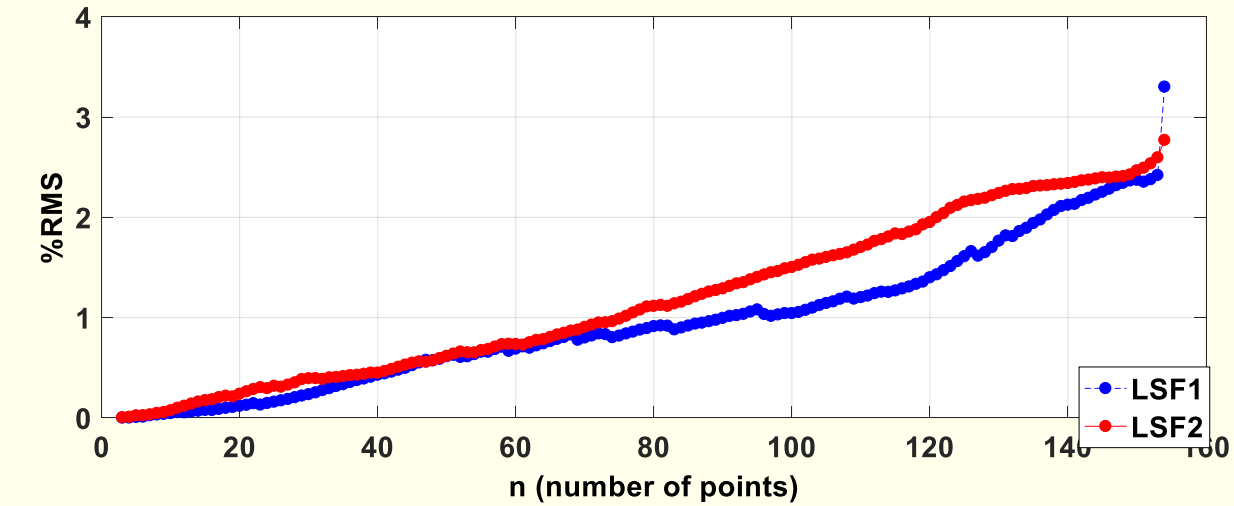
Method 1 (LSF1):

Linear regression $y = ax + b$ with $y = dSCD$ and $x = AMF$

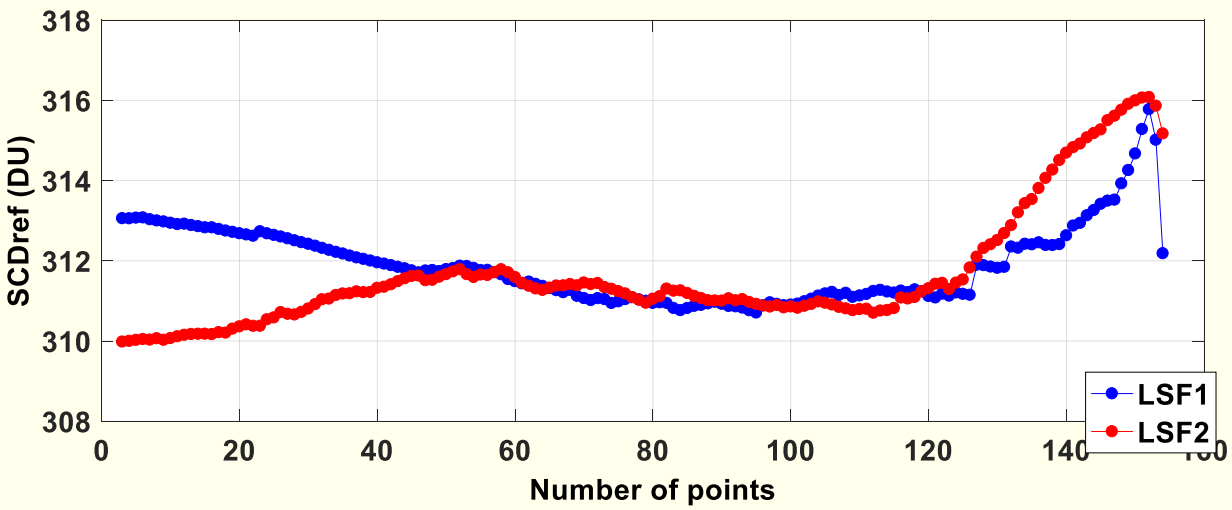
Method 2 (LSF2):

Linear regression $\frac{y}{x} = a + \frac{b}{x}$ with $\frac{y}{x} = \frac{dSCD}{AMF}$ and $\frac{1}{x} = \frac{1}{AMF}$

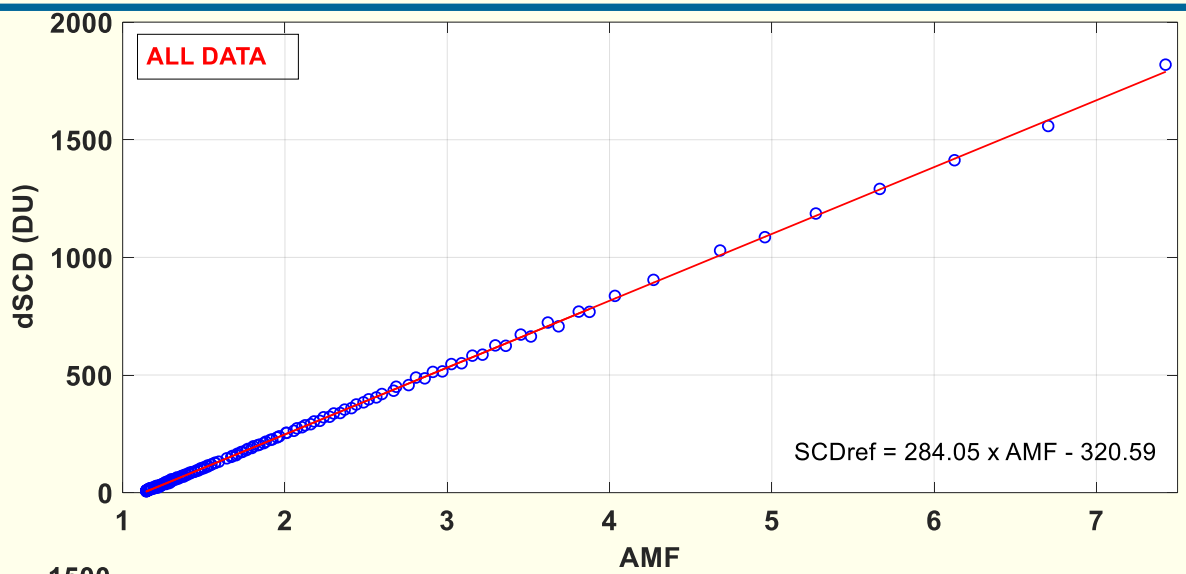
Outlier removal based on RMS error

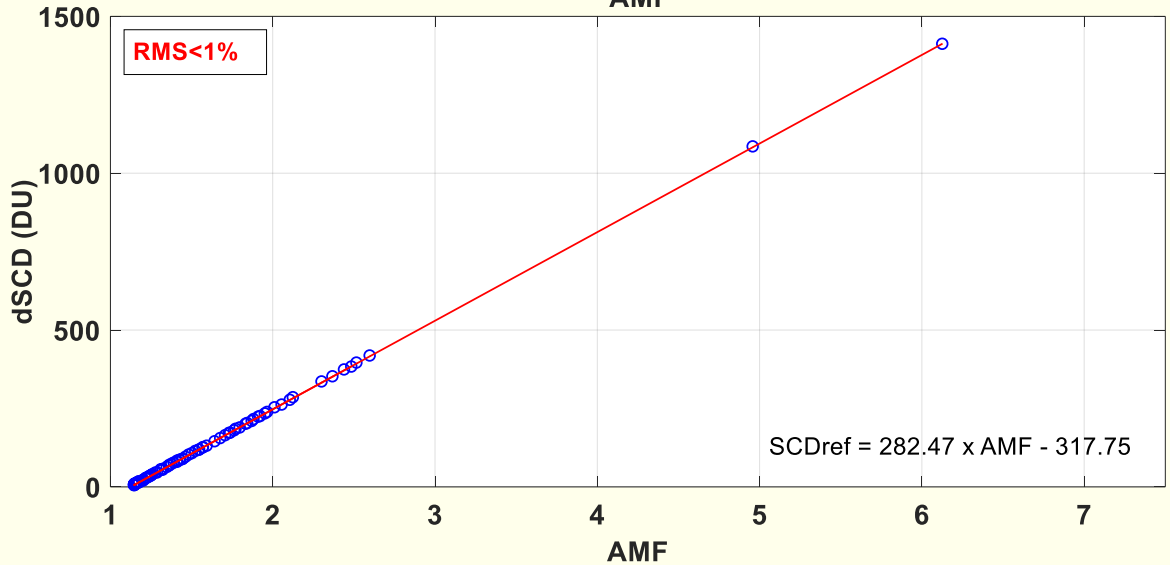


$$RMS\% = \frac{RMS}{dSCD} \times 100$$

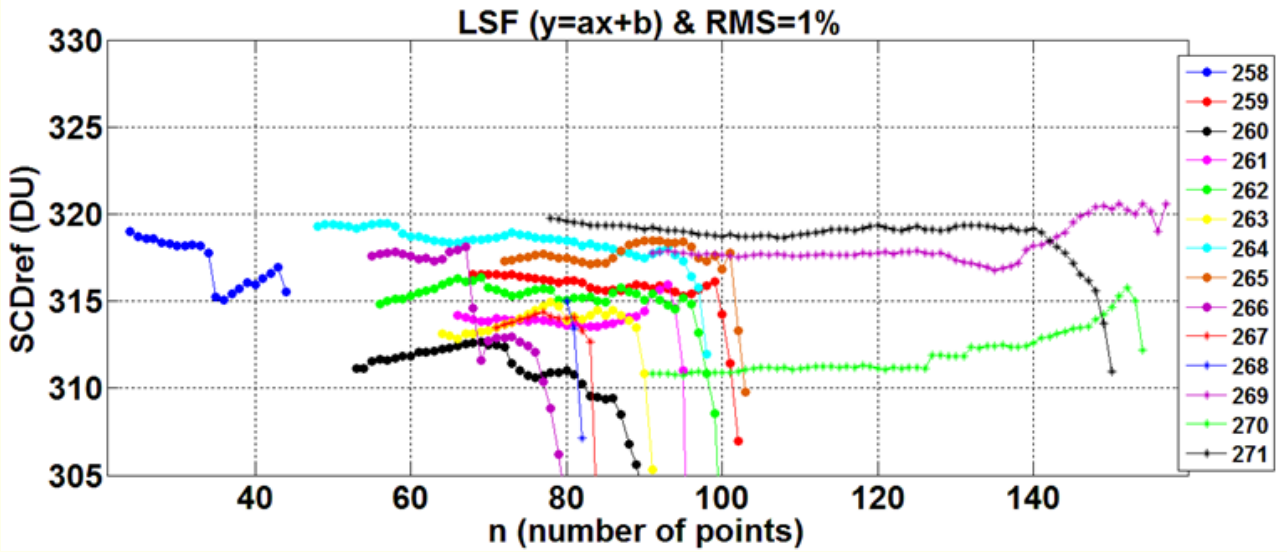


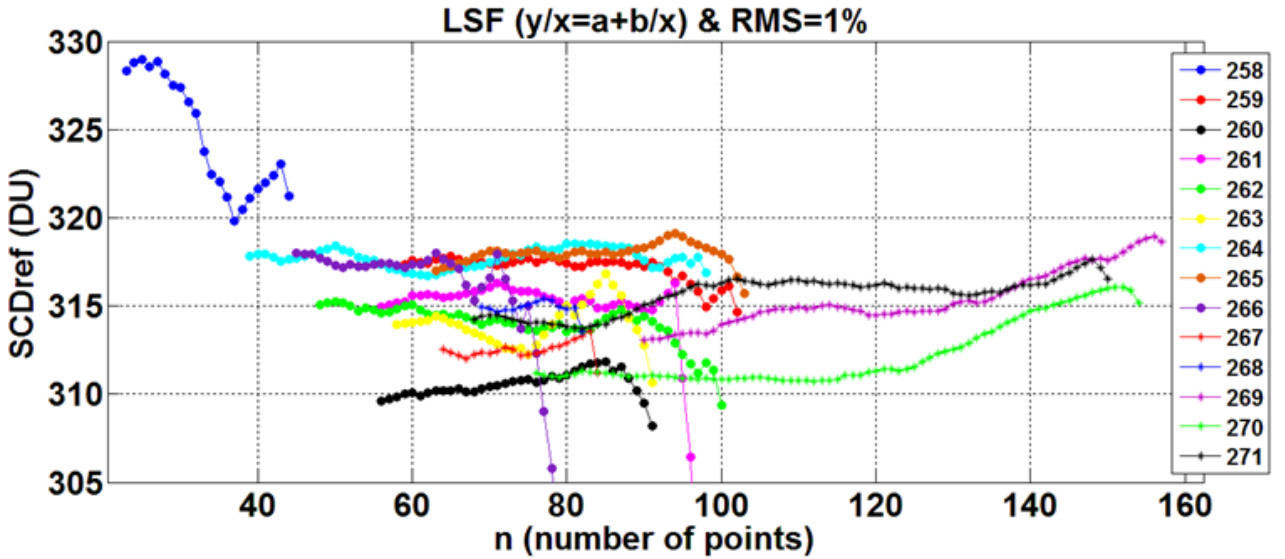
Langley plots Izaña





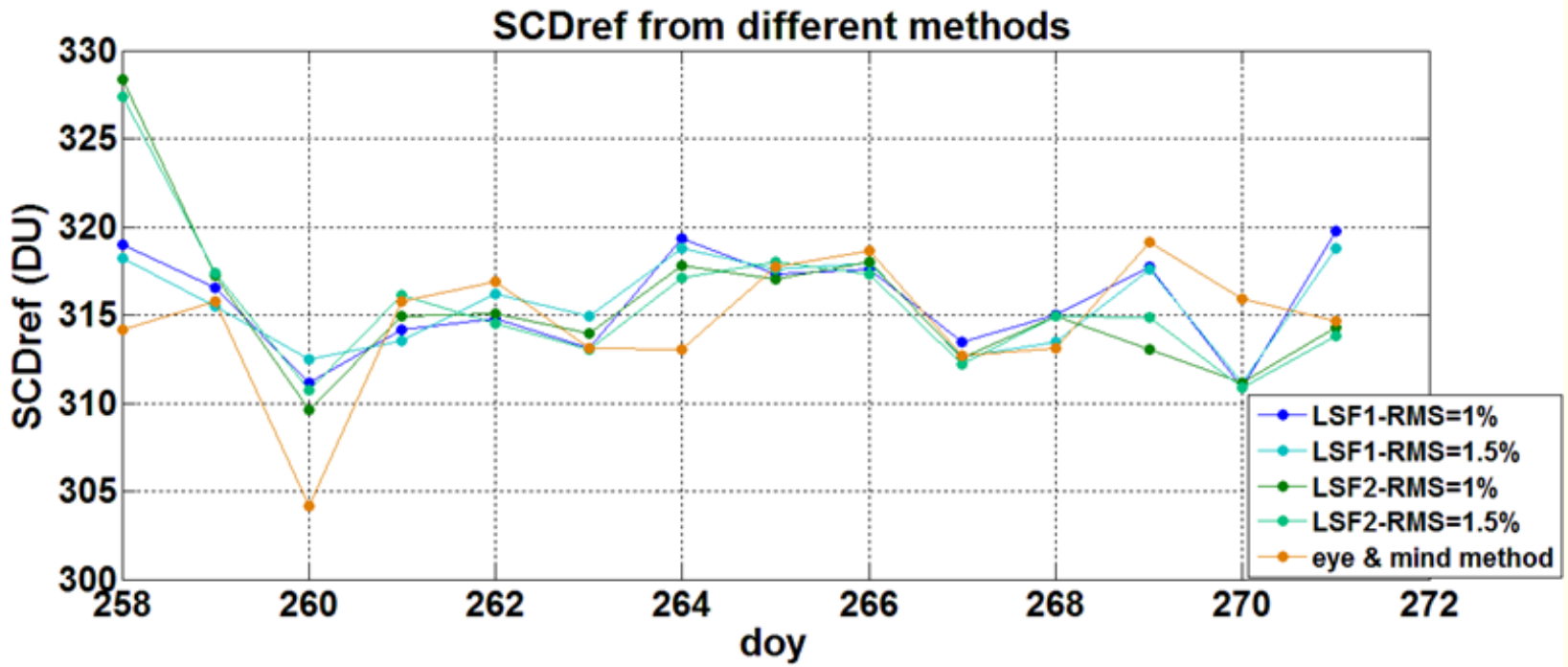
SCD_{REF} estimation





LAP-AUTH

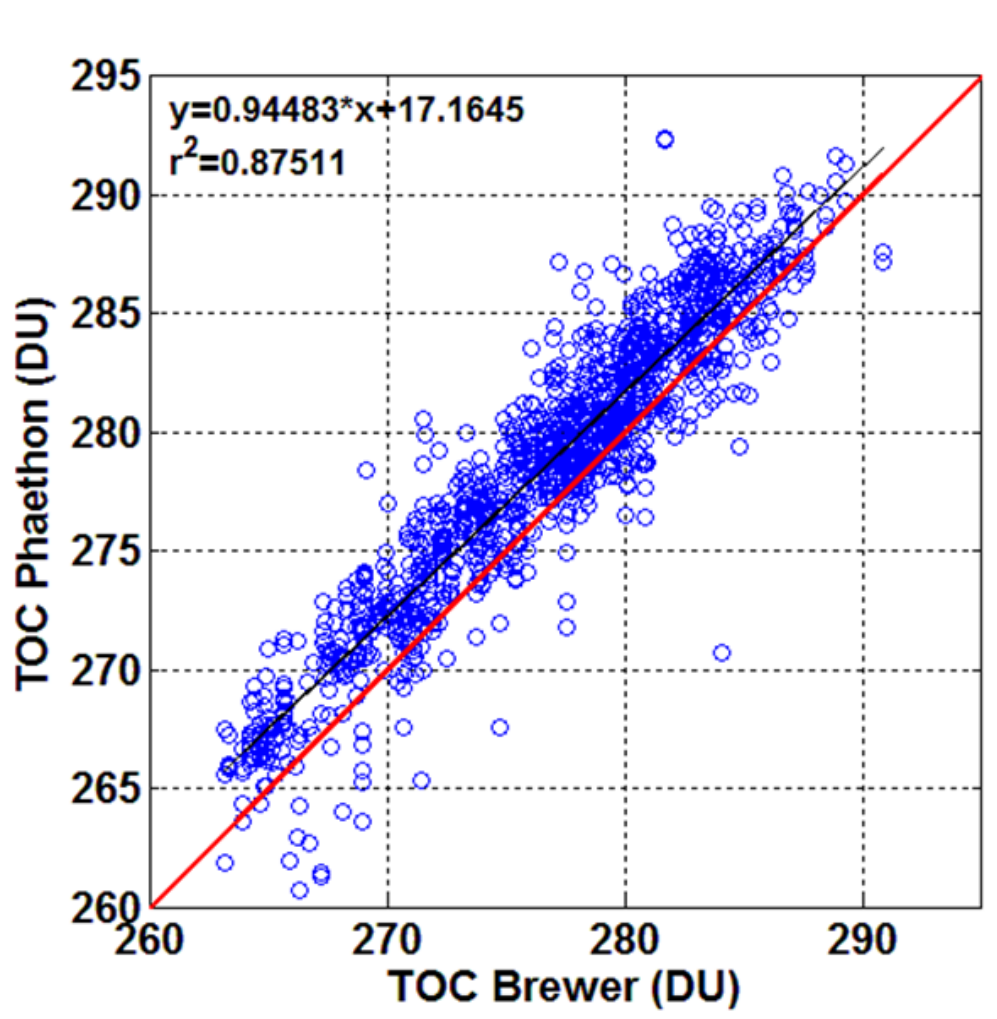
Estimated SCD_{REF} for different days/methods



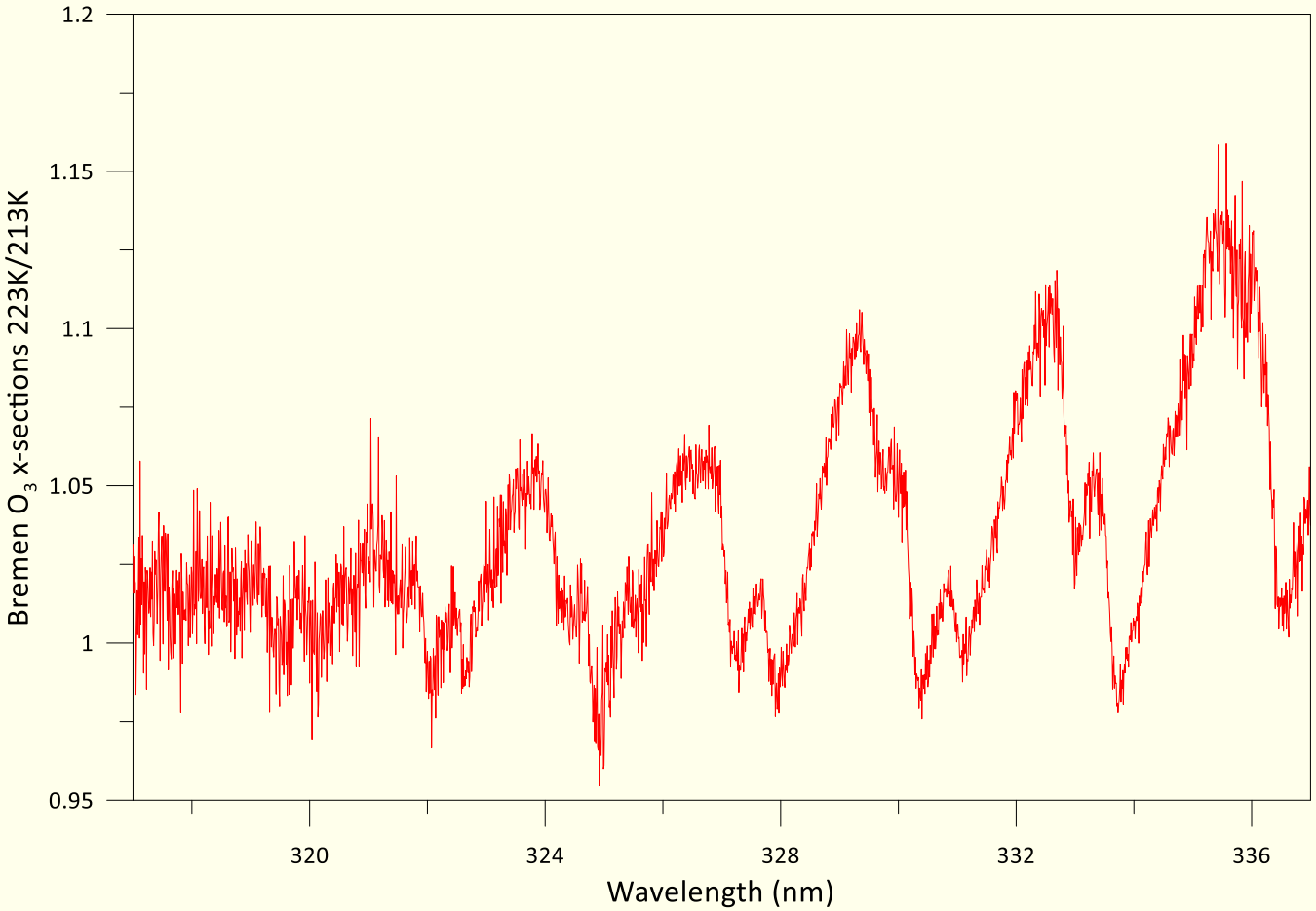
- LSF1: 315.7 DU
- LSF2: 315.6 DU
- “eye and mind” 314.6 DU

Phaethon vs Brewer #183 – Izaña campaign

- ✓ Small variation of TOC during the campaign (~30 DU) increases the uncertainty of the regression (r^2=0.87)
- ✓ Phaethon overestimates TOC by **~0.7±0.8 %** (~2 DU)
- ✓ Phaethon TOC is likely dependent on stratospheric temperature since in the DOAS retrieval all wavelengths in the range 315-337 nm are used

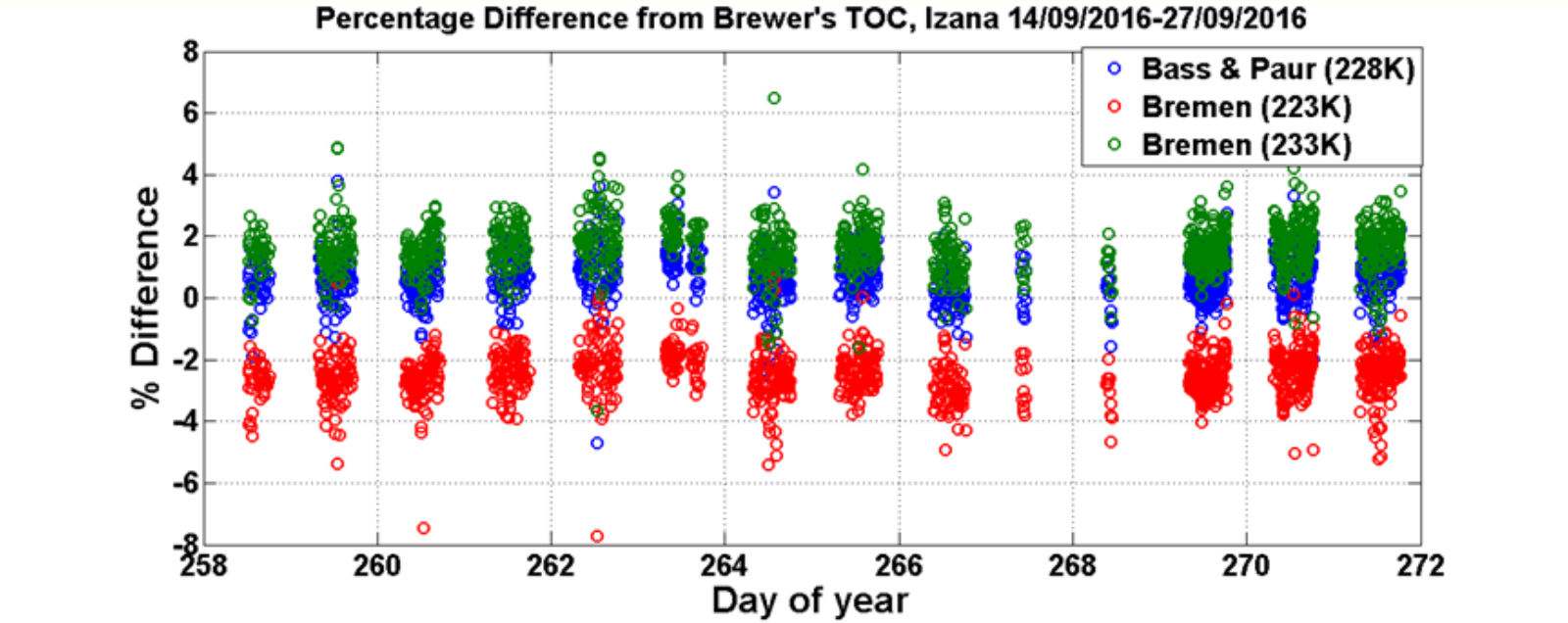


Temperature effect on O_3 x-sections



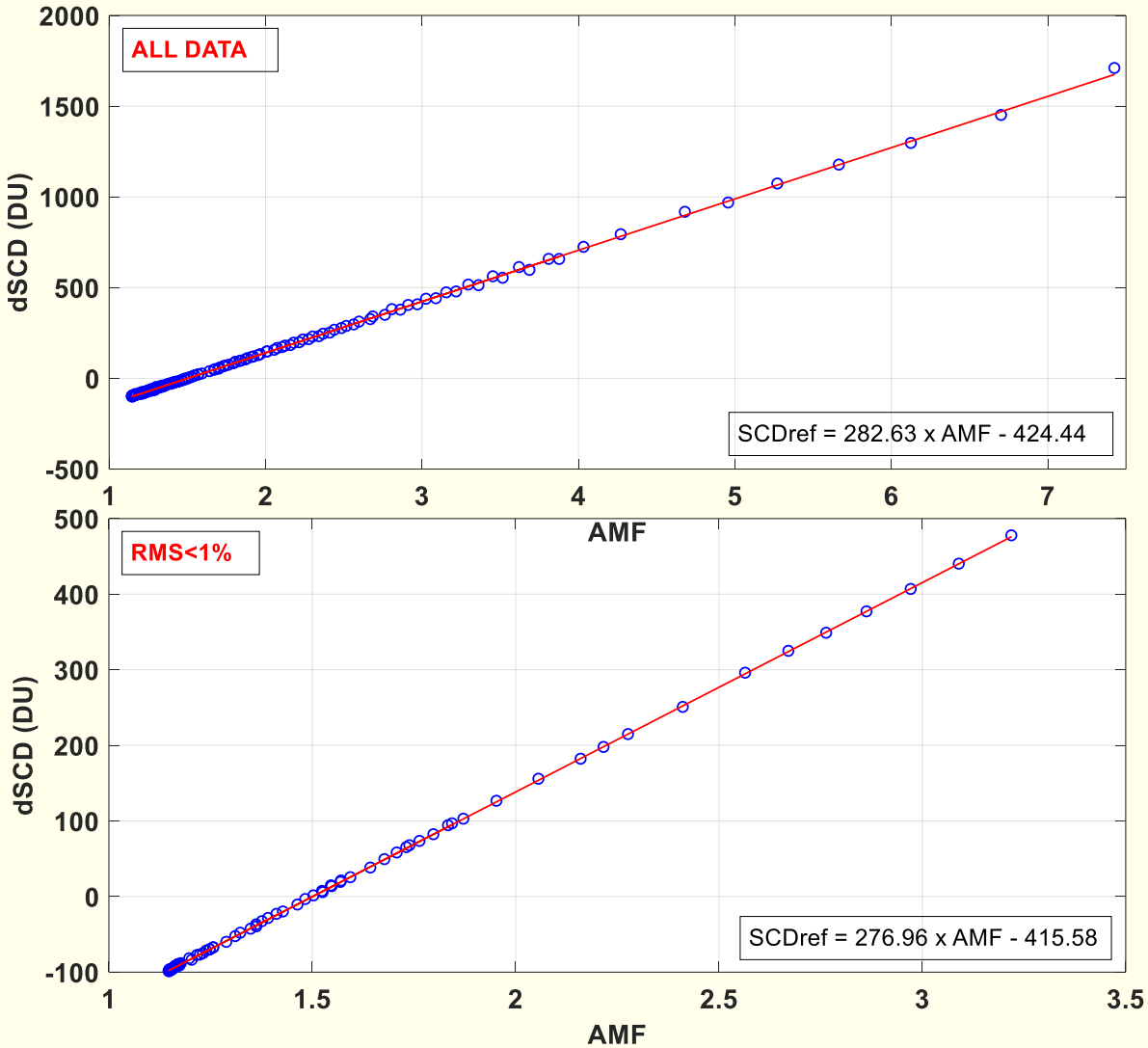
Effect of O_3 x-sections on Phaethon TOC

Phaethon vs Brewer 183 (BP based)

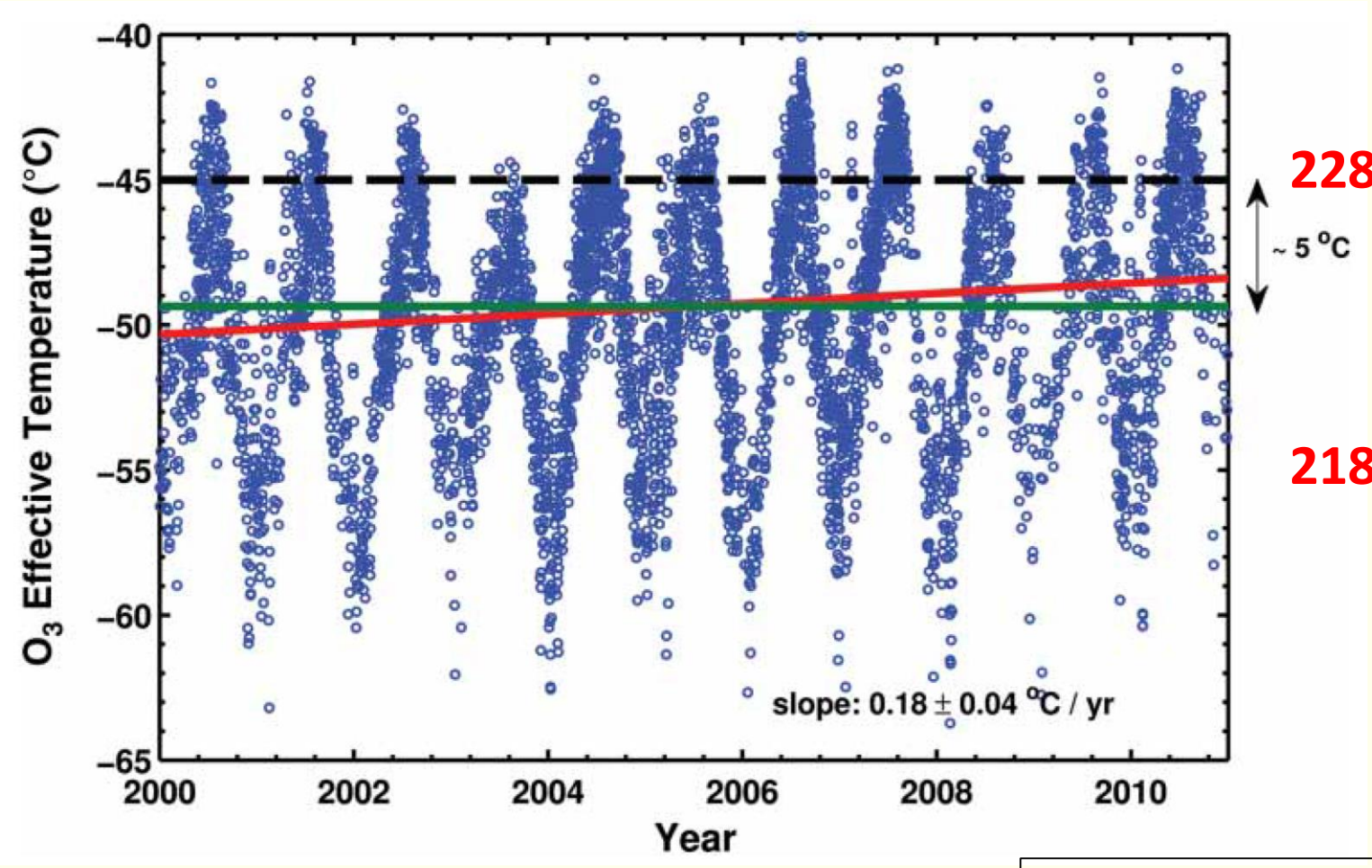


O_3 absorption cross-section	Mean difference (%)	Std (% difference)
Bass & Paur (228K)	0.69	0.78
Bremen (223K)	-2.47	0.77
Bremen (233K)	1.65	0.79

SCD_{REF} for Thessaloniki



Effective ozone temperature in Thessaloniki

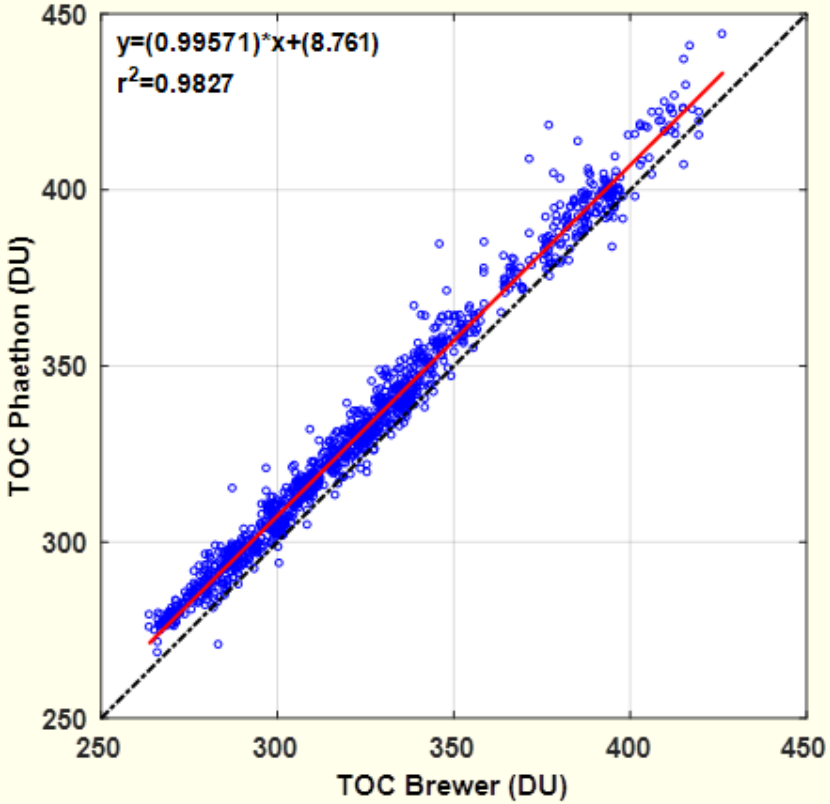


Fragkos et al., 2013

Phaethon vs Brewer #005 - Thessaloniki

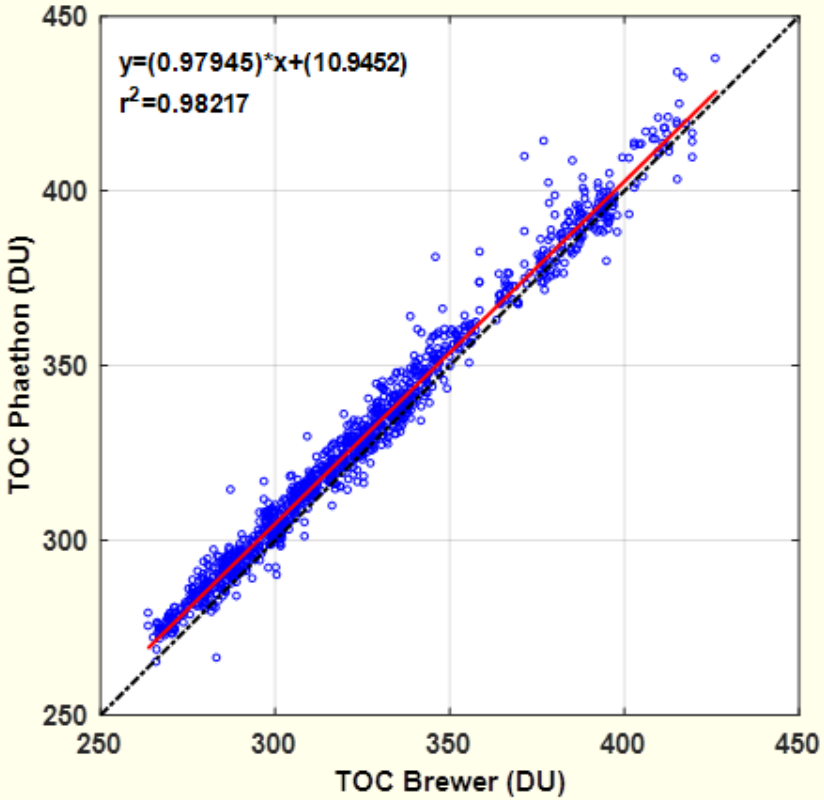
- Cold-period data (October 2015 – March 2017)

Paur & Bass 228 K



bias 3 DU (0.9±2.7 %)

Paur & Bass 218 K

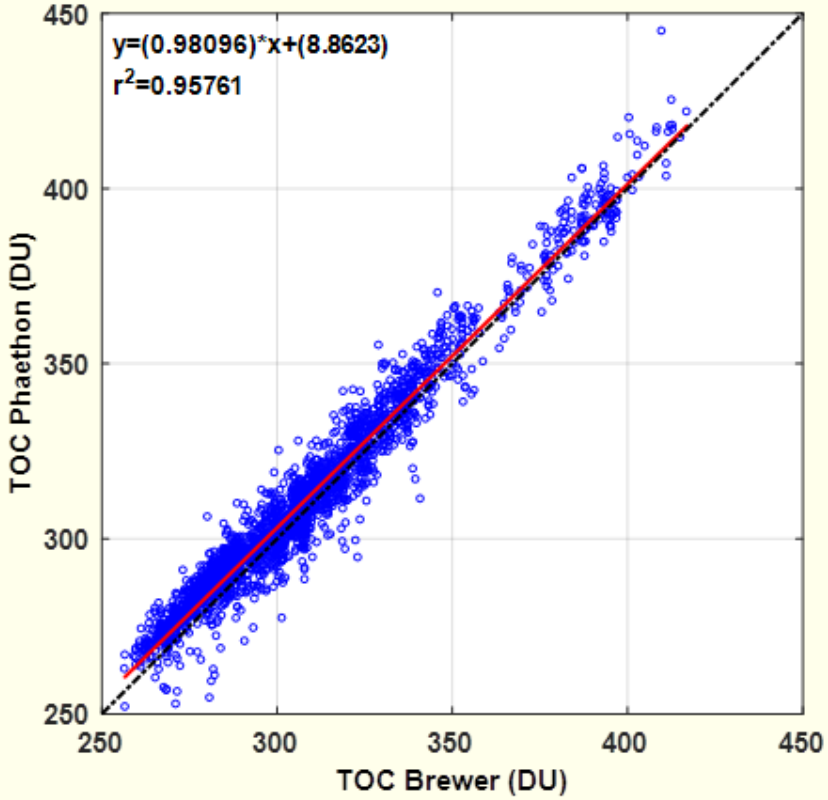


bias 0.8 DU (0.2±2.4 %)

Regular spectra (without short pass filter)

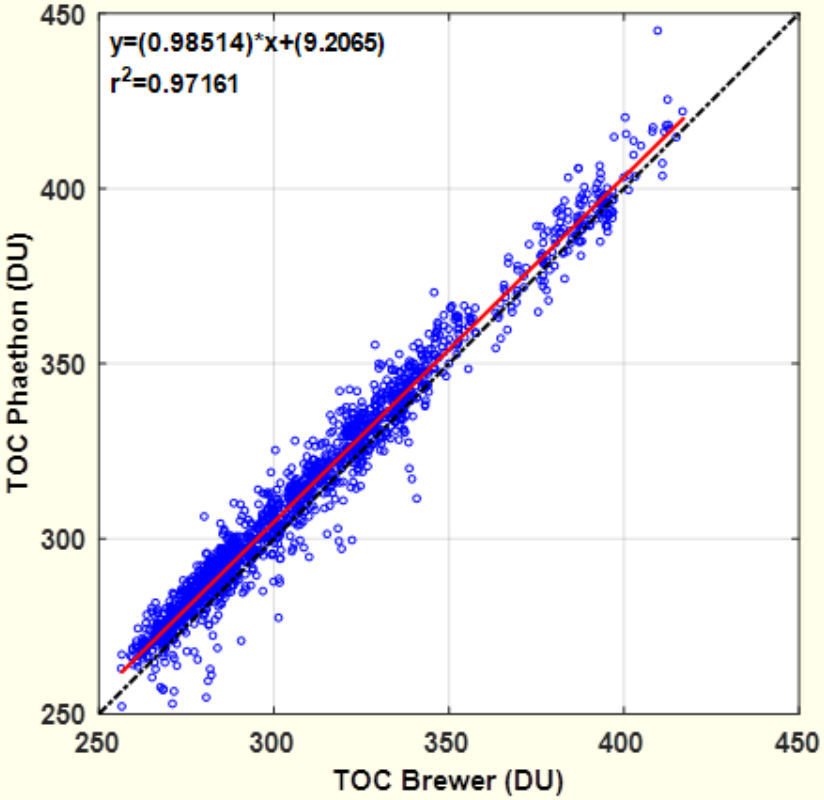
- October 2015 – March 2107 **(Paur & Bass 218 K)**

All data



bias 0.2±2.1 %

Cold period



bias 0.5±2.1 %

Uncertainty estimation of Phaethon TOC

- Factors contributing:
  - Spectral direct radiance measurements (very small)
  - spectral characteristics of the measured spectra (mainly due to noise)
  - DOAS analysis
- Systematic uncertainties due to cross-section datasets of O_3 (& other absorbers)
  - Average bias in BP-based *dSCD* relative to Bremen ~**1.5%** and BDM **~1%** (independent of SZA but increasing with decreasing *dSCD*)
- Random uncertainty of the DOAS analysis: on average **2.7%** in the *dSCD*
  - Effects on TOC are much smaller, due to division by the AMF
- Uncertainty in the SCD_{REF} **~0.1%**
  (estimated from the Langley regressions of the 14-day campaign in Izaña)
- Combined uncertainty of the respective vertical column densities:

$$\sigma_{total}^2 = \frac{\sigma_{dSCD}^2}{AMF^2} + \frac{\sigma_{SCD_{REF}}^2}{AMF^2} = \frac{\sigma_{dSCD-systematic}^2}{AMF^2} + \frac{\sigma_{dSCD-random}^2}{AMF^2} + \frac{\sigma_{SCD_{REF}}^2}{AMF^2}$$

- Average total uncertainty: **2.7%** (for large slant columns reduced to **0.9%**)

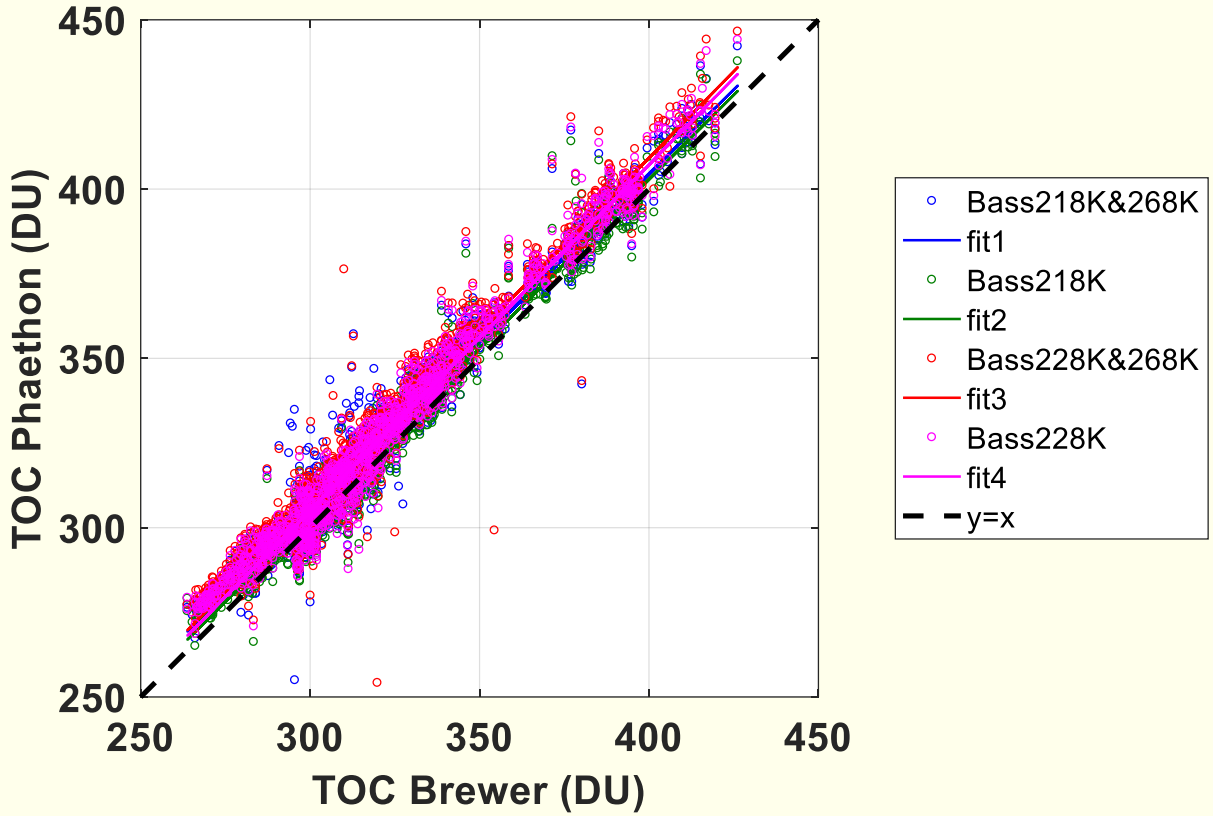
DOAS retrieval with different temperature combinations

y1=(0.9927)*x1+(7.4739)
$r1^2$=0.93515

y2=(0.99776)*x2+(3.7474)
$r2^2$=0.97424

y3=(1.0237)*x3+(-0.31841)
$r3^2$=0.94922

y4=(1.0211)*x4+(-1.2399)
$r4^2$=0.97057



Conclusions

- Langley plots of the Izaña campaign dataset are used to derive the slant column of the reference spectrum used in the DOAS analysis for TOC retrieval
- The same dataset can be used for reference spectra recorded with the same spectrometer at other locations and times
- Total ozone data derived from Phaethon in Thessaloniki compare well with Brewer #005 (on average within 1%)
- Phaethon TOC shows higher noise compared to Brewer
- A small effect appears in TOC (~ 0.7 %) when BP cross-sections at different temperatures (218 vs 228 K) are used, implying a seasonal dependence in the derived TOC.

Thank you for your attention!