CO Total Column Retrieval from SCIAMACHY: Full-Mission Validation with NDACC and TCCON

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Introduction

Space-borne (s-b) instruments such as the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) measuring the composition of the Earth's atmosphere ask for sufficient validation. Considerable effort has been invested in establishing ground-based (g-b) validation infrastructure such as the Network for the Detection of Atmospheric Composition Change(NDACC) or the Total Carbon Column Network (TCCON).

SCIAMACHY . . .

- observed the scattered and reflected solar spectral radiance transmitted through the atmosphere from the ultra violet (UV) to short wave infrared (SWIR) spectral range
- Channel 8 observed radiance in the SWIR range from 2259.38 nm to 2386.07 nm (4426 – 4191 cm^{-1})

Accurate retrieval of CO from SCIAMACHY Channel 8 is demanding because of . . .

- low optical depth of CO compared to the total optical depth
- temporal degradation of the detector affecting throughput
- amount of dead and bad pixels ($\approx$ 50 pixels utilized for retrieval from 4280 to 4305 cm^{-1} (Lichtenberg et al. 2010))

BIRRA - Beer InfraRed Retrieval Algorithm

- Forward – SWIR radiative transfer – Intensity $\mathcal{I}$ vs. wavenumber ν

$$\widehat{I}(\nu) \;=\; \frac{r(\nu)}{\pi}\mu_{\odot} I_{\text{sun}}(\nu) \,\times\, \exp\left(-\sum_m \alpha_m \, \tau_m(\nu)\right) \,\otimes\, \mathcal{S}(\nu,\gamma) \,+\, b(\nu) \qquad (1)$$

$$\tau_m(\nu) \;=\; \int_{\uparrow\downarrow} \mathrm{d}z \left(\frac{1}{\mu} + \frac{1}{|\mu_{\odot}|}\right) n_m^{\text{ref}}(z)\, k_m(\nu, z) \qquad (2)$$

α_m scaling factor (in this work CO, CH_4, H_2O)
n_m molecular number density; k_m absorption cross section
$\mathcal{S}$ spectral response function (SRF); θ SZA; **b** baseline

- Inversion: separable least squares fit
  State vector $\boldsymbol{x} = (\alpha, \beta)$ of nonlinear (molec. scaling factors) and linear (reflectivity **r**, baseline **b**) parameters
- BIRRA – two versions:
  - 'scientific prototype version' (this work!)
  - operational $\in$ SCIAMACHY level 1b-2 processor (v7.0)

CO from SCIAMACHY and Ground-Based Networks

SCIAMACHY

- Calibrated spectra normalized by SCIA sun measured spectrum
- Actual dry air volume mixing ratio (VMR) f for CO:

$$f_{\text{CO}} = \frac{\alpha_{\text{CO}}}{\alpha_{\text{CH4}}} f_{\text{CO}}^{\text{ref}} \qquad (3)$$

NDACC

- CO and CH_4 from mid IR (unlike SCIA)
- some dozen stations, mostly operational for 2 decades

$$f_{\text{CO}} = N_{\text{CO}} \left(\frac{p}{m_{\text{air}}\, g} - N_{\text{H2O}} \frac{m_{\text{H2O}}}{m_{\text{air}}}\right)^{-1} \qquad (4)$$

TCCON

- CO and CH_4 from near IR (like SCIA)
- most stations operational only in the last decades (few data for early SCIA years)

$$f_{\text{CO}} = 0.2095 \frac{N_{\text{CO}}}{N_{\text{O2}}}. \qquad (5)$$

Validation Methodology

Validation means . . .

- assessing the performance of a system against some equivalent information that is regarded as 'truth' reference (Einarsson 2005)
- qualifying differences due to errors in the acquisition or retrieval process, i.e. instruments or algorithms performance

An appropriate validation strategy therefore considers . . .

- the mismatch of s-b and g-b measurements in time and space
- the different volume of air both address
- therefore, the incorporation of non-instrumental comparison errors

A representative (optionally weighted with respect to time τ and space ρ) average value μ and std. deviation σ for both, s-b and g-b data was hence defined according to:

$$\mu \;=\; \frac{\sum \tau\, \rho\, \psi}{\sum \tau\, \rho} \qquad\qquad \sigma = \sqrt{\frac{\sum \tau\, \rho\, (\psi - \mu)^2}{\sum \tau\, \rho}}\,. \qquad (6)$$

Summary

- spatial and temporal averaging is required
- trade-off between incorporating high-quality observations and temporally & spatially representative ones for comparison (Fig. 1, 3 and 4)
- linear weighting gives slightly better agreements (Fig. 1 and 3)
- goodness of agreement w.r.t. NDACC or TCCON depends on the reference site (Fig. 2)
- most SCIAMACHY CO values agree within std. dev. of the g-b observations

References & Further Information

- Borsdorff, T., P. Tol, J. E. Williams, J. de Laat, J. van de Brugh, P. Nédélec, I. Aben, and J. Landgraf, 2016: Carbon monoxide total columns from SCIAMACHY 2.3 μm atmospheric reflectance measurements: towards a full-mission data product (2003–2012). *Atmos. Meas. Tech.*, **9**, 227-248, doi:10.5194/amt-9-227-2016.
- Gimeno García, S., F. Schreier, G. Lichtenberg, and S. Slijkhuis, 2011: Near infrared nadir retrieval of vertical column densities: methodology and application to SCIAMACHY. *Atmos. Meas. Tech.*, **4**, 2633-2657, doi:10.5194/acp-9-3799-2009.
- Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, C. Liu, D. G. Feist, and P. O. Wennberg, 2015: The Total Carbon Column Observing Network's GGG2014 Data Version. Tech. Report, 42 pp, doi:10.14291/tccon.ggg2014.documentation.R0/1221662.

Results of the CO Validation

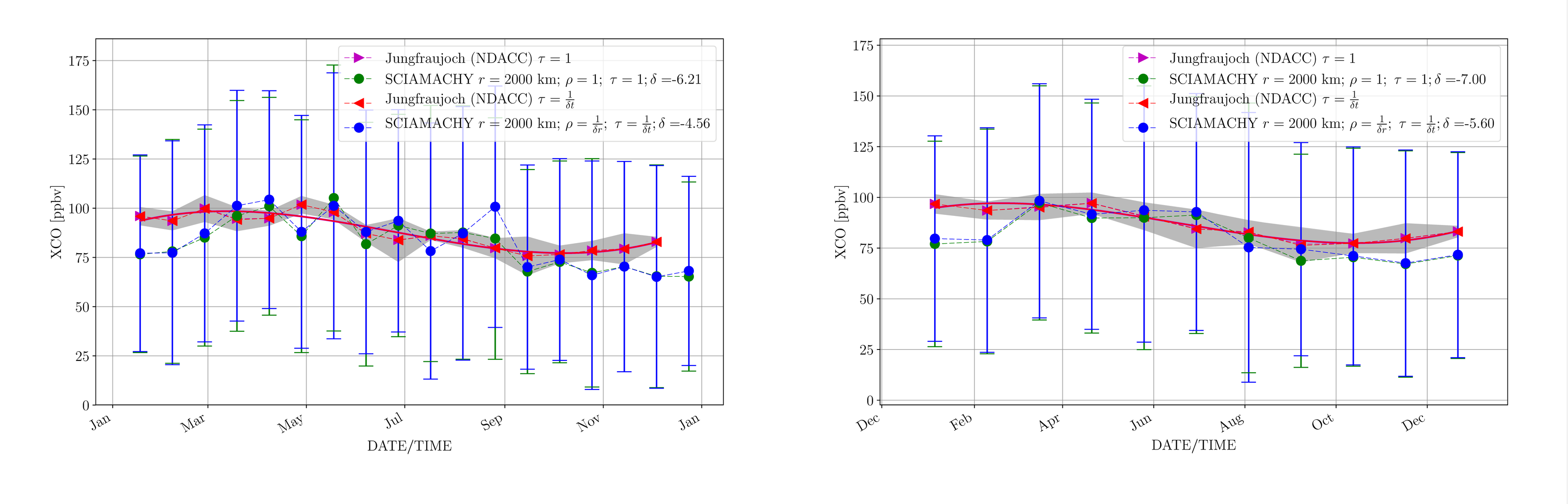

Figure 1 - Effect of weighting: *CO mixing ratios (linear weighting and no weighting), incorporating s-b observations within 2000 km from Jungfraujoch in the year 2003.* $\delta = \bar{\mu}_{\text{sb}} - \bar{\mu}_{\text{gb}}$ *in parts per billion in volume (ppbv). Left: 20 days average. Right: 35 days average.*

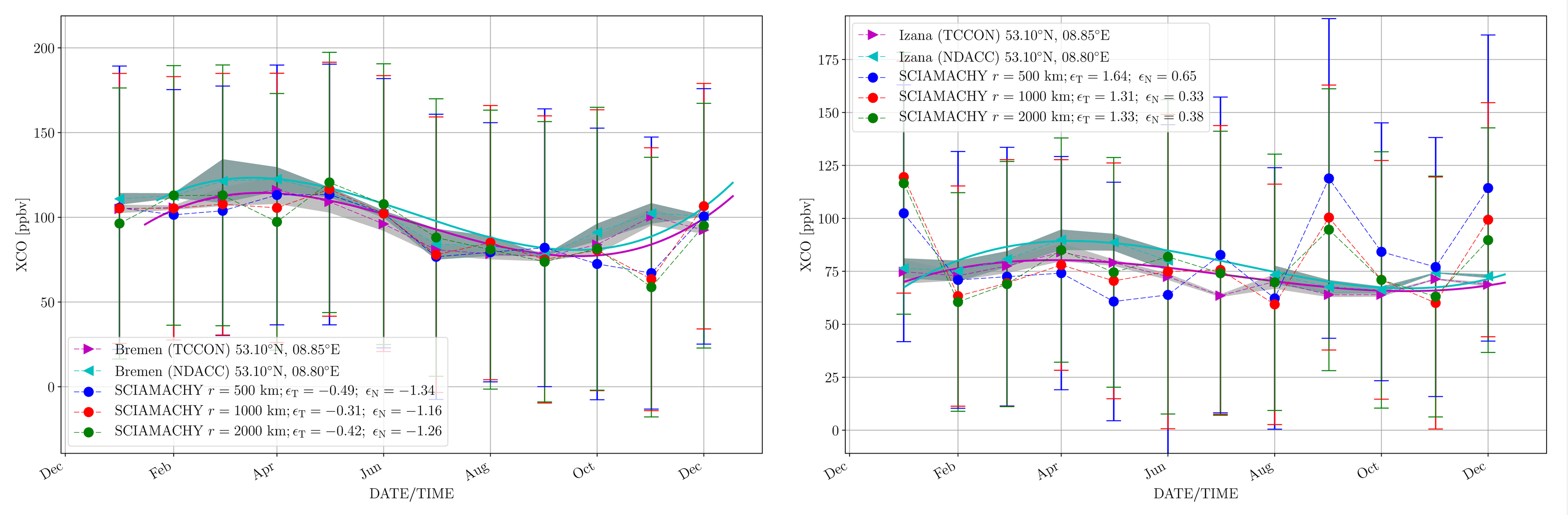

Figure 2 - NDACC and TCCON: *Varieties in averaged CO VMR's between both networks at the same reference site. No weighting applied; the standardized residual* $\epsilon = \sum \frac{\bar{\mu}_{\text{sb}} - \bar{\mu}_{\text{gb}}}{\sigma_{\text{sb}}}$. *Left: Bremen in 2007. Right: Izana in 2009.*

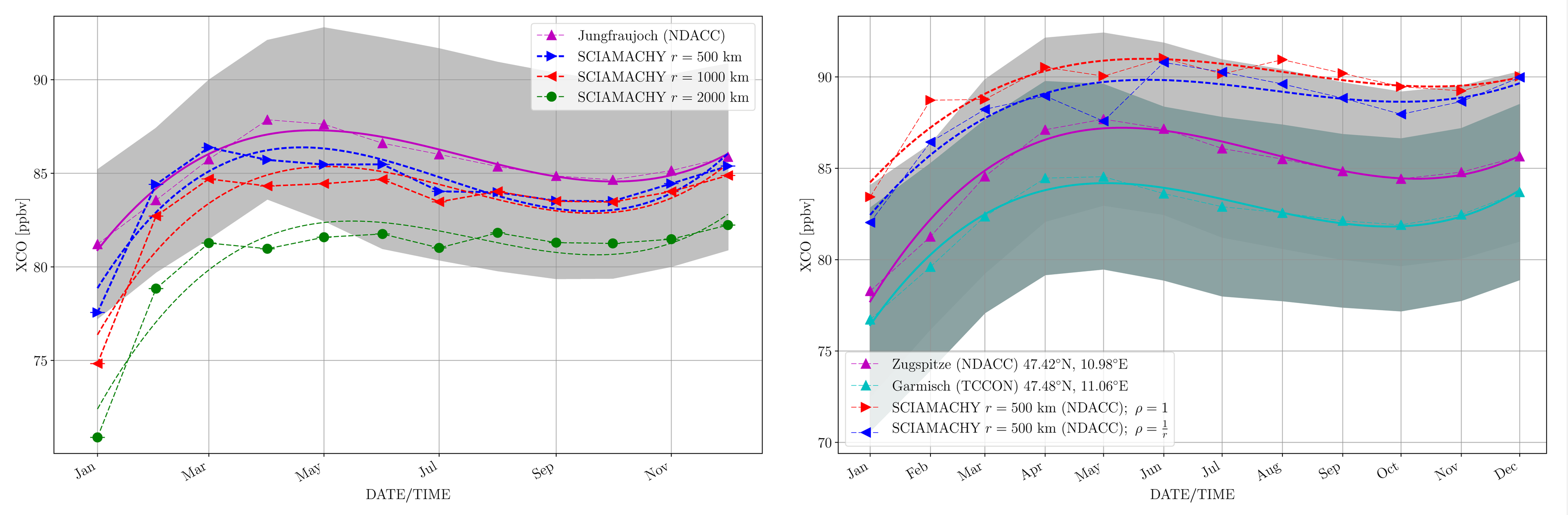

Figure 3 - Multiannual averages: *Annually linear detrended averages for three different g-b reference sites. An individual measurement can be represented according to* $\psi_i = a_0 + a_1 t_i + \epsilon_i$. *Left: Jungfrauhoch (*$\delta = -0.51$*) full-mission data from 2003 – 2011; no weighting applied. Right: Garmisch (*$\delta = 6.87$*) and Zugspitze (*$\delta = 4.60$*) from 2007 – 2011; weighted and unweighted approach. The number of measurements within each year ranges from roughly 2000 to 8000 for* $r = 500$ km *around Zugspitze.*

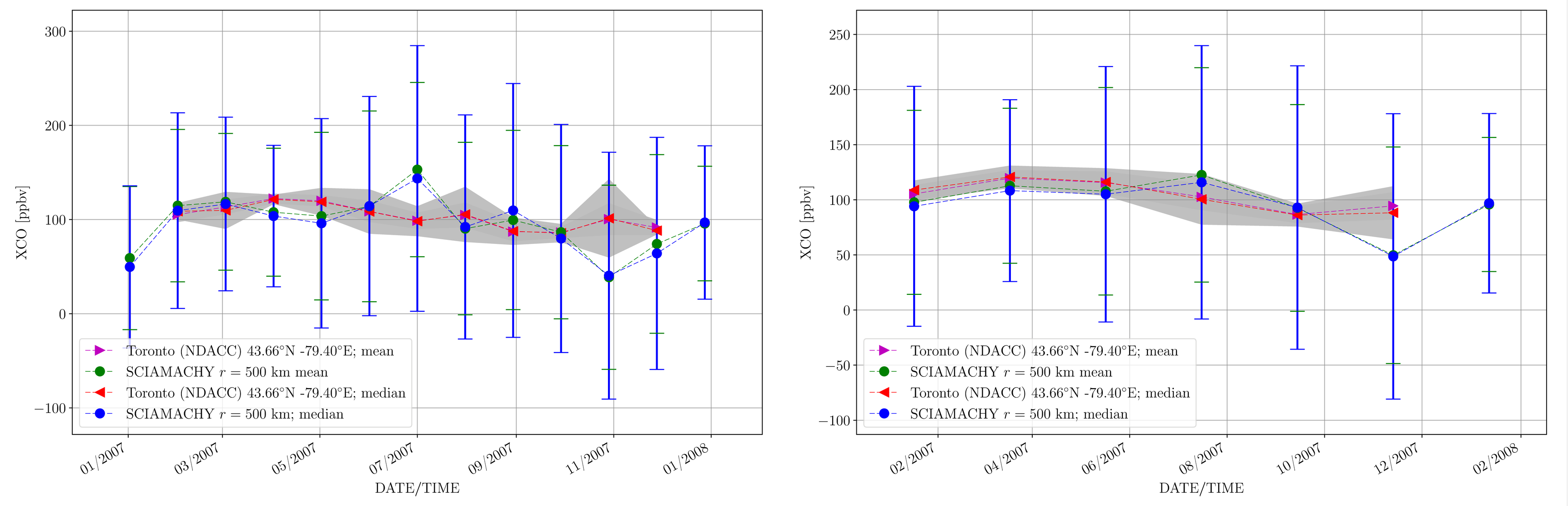

Figure 4 - Mean vs. median: *In case of median, instead of the std. deviation the inter quartile range Q3 - Q1 is given. Left: Toronto with a time step of 30 days. Right: Same reference site but using a time step of 60 days.*

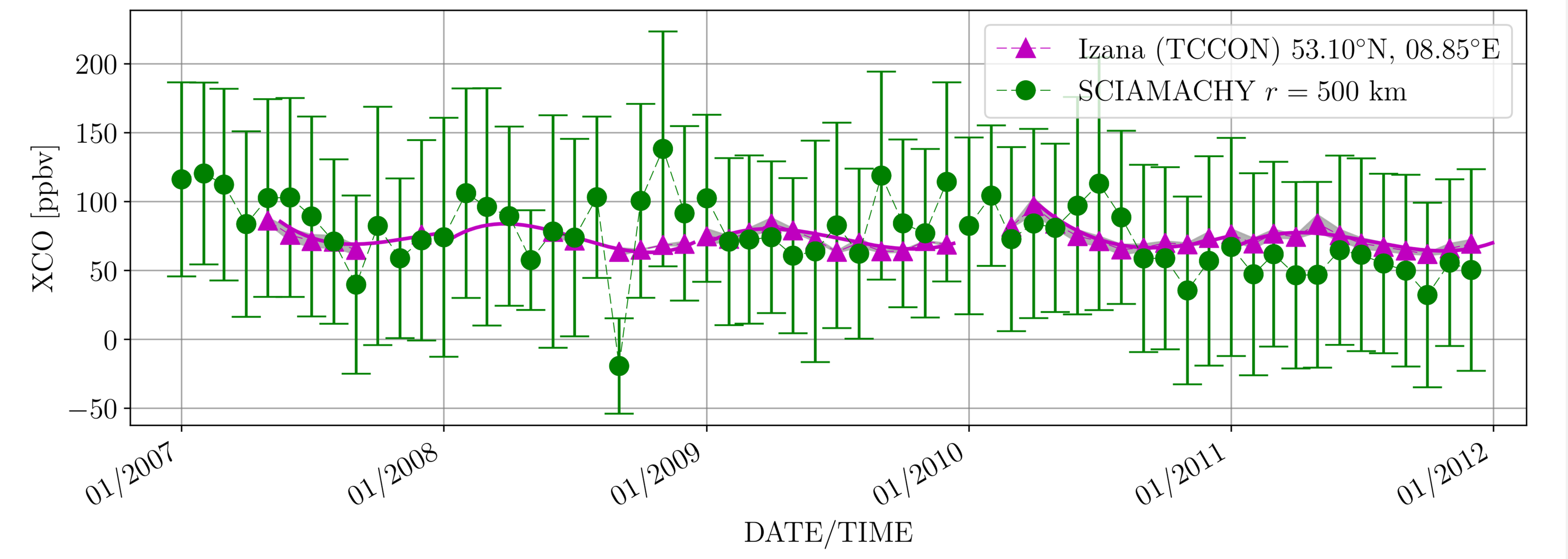

Figure 5 - Time series: *Month mean averages for Izana. Standardized residuals for the years 2007 – 2011 yield* $\epsilon = \{0.41, -0.52, 1.64, -0.25, -3.15\}$*, respectively.*