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Advanced retrieval of SO_2 from TROPOMI using COBRA

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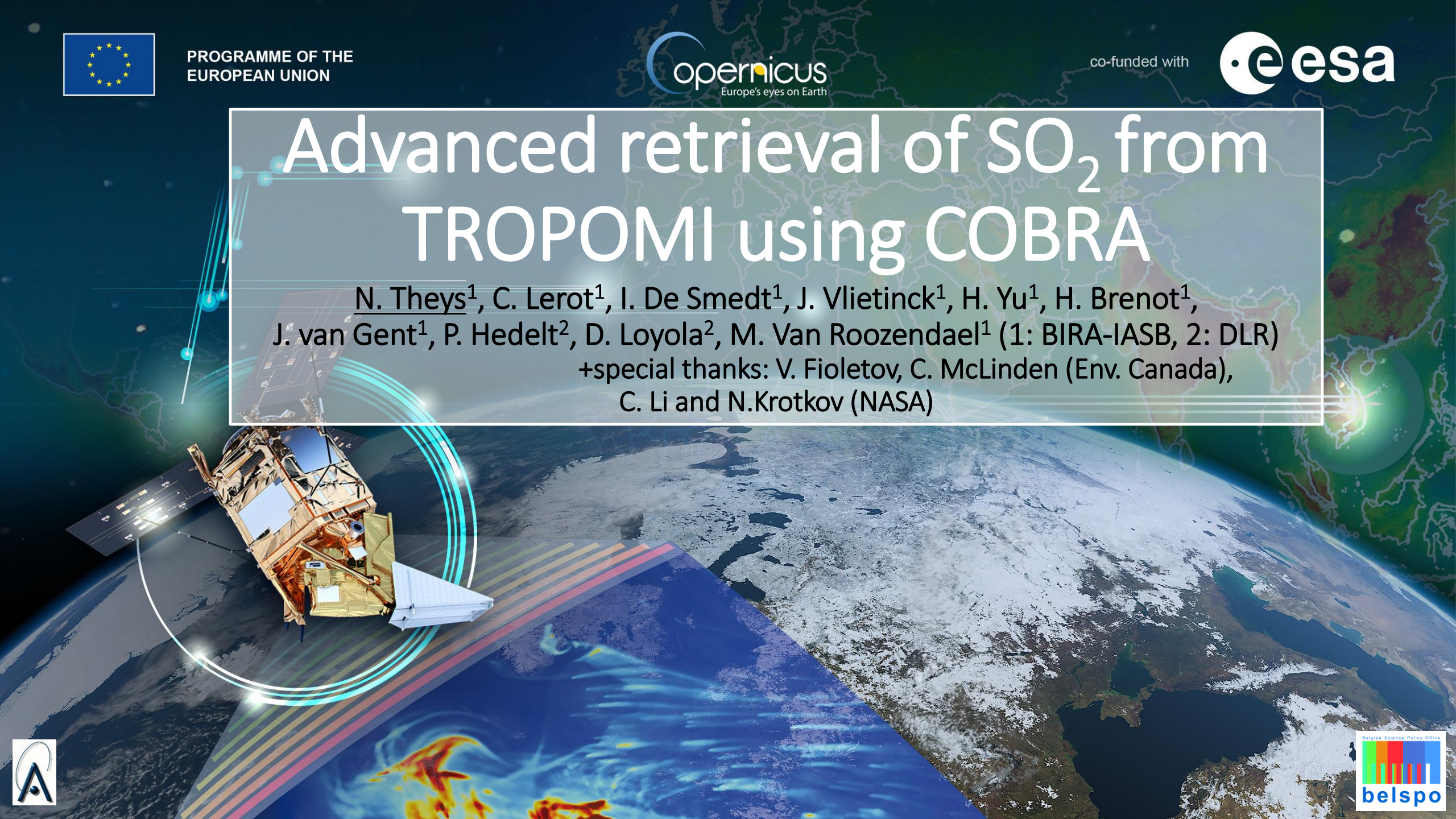
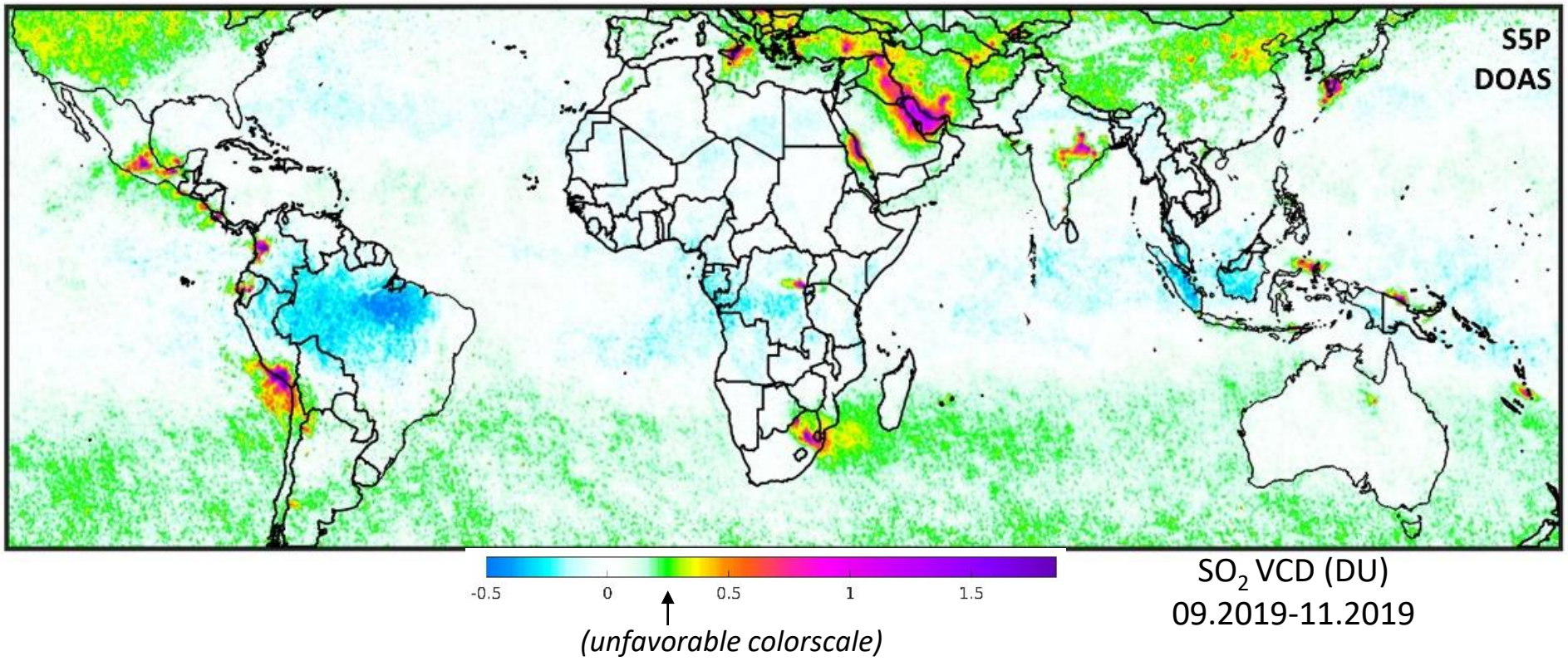
+special thanks: V. Fioletov, C. McLinden (Env. Canada), C. Li and N.Krotkov (NASA)



belspo

Motivation

Weak emission sources are difficult to study with current TROPOMI SO_2 product because of large scale biases (~0.2 DU), in part due to imperfect Ring correction.



=> Need for alternative retrieval approach

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Retrieval methods

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DOAS (Diffential Optical Absorption Spectroscopy)

$y = K.x + \epsilon$

(linearized form)

y: -log(I/Io) (I, Io: wvl calibrated spectra)
K: cross-sections + other spectra
x: SCDs + other fit parameters
ϵ: measurement error

$$\longrightarrow \quad \hat{x} = (K^T S_\epsilon^{-1} K)^{-1}.K^T S_\epsilon^{-1}.y$$

Main disadvantage: *K* is uncertain and spectral interferences not well controlled even after settings optimization.

Note: most often, S_ϵ is diagonal and proportionnal to unity matrix (unweighted fit).

COBRA (Covariance-based retrieval algorithm)

(based on previous work on IASI: Walker et al. 2011, doi:10.5194/amt-4-1567-2011)

$y = \underbrace{y_{SO2}}_{k.SCD} + y_{bck} + \epsilon$

k: (vector) cross-section of SO_2.
y_{bck}: -log(I/Io) without contribution from SO_2

$$\longrightarrow \quad \boxed{\widehat{SCD} = (k^T S^{-1} k)^{-1}.k^T S^{-1}.(y - \bar{y})}$$

Assumption: y_{bck} + ϵ can be considered as an error term, characterized by a mean spectrum $\bar{y}$ and an error covariance matrix S (pdf Gaussian distribution)
=> S and $\bar{y}$ are obtained from a set of SO_2-free measured spectra

Implementation (Theys et al., ACP, 2021)

- S (and $\bar{y}$) is calculated for each TROPOMI row (450), per orbit and for 6 along-track segments.
- Iterative estimation of S by excluding pixels with |SNR|>1.5

$$SNR = \frac{k^T S^{-1}.(y - \bar{y})}{\sqrt{k^T S^{-1} k}}$$

COBRA generalizes the Principal Component Analysis (PCA) algorithm (Li et al., 2013, 2017)

TROPOMI SO_2 products comparison

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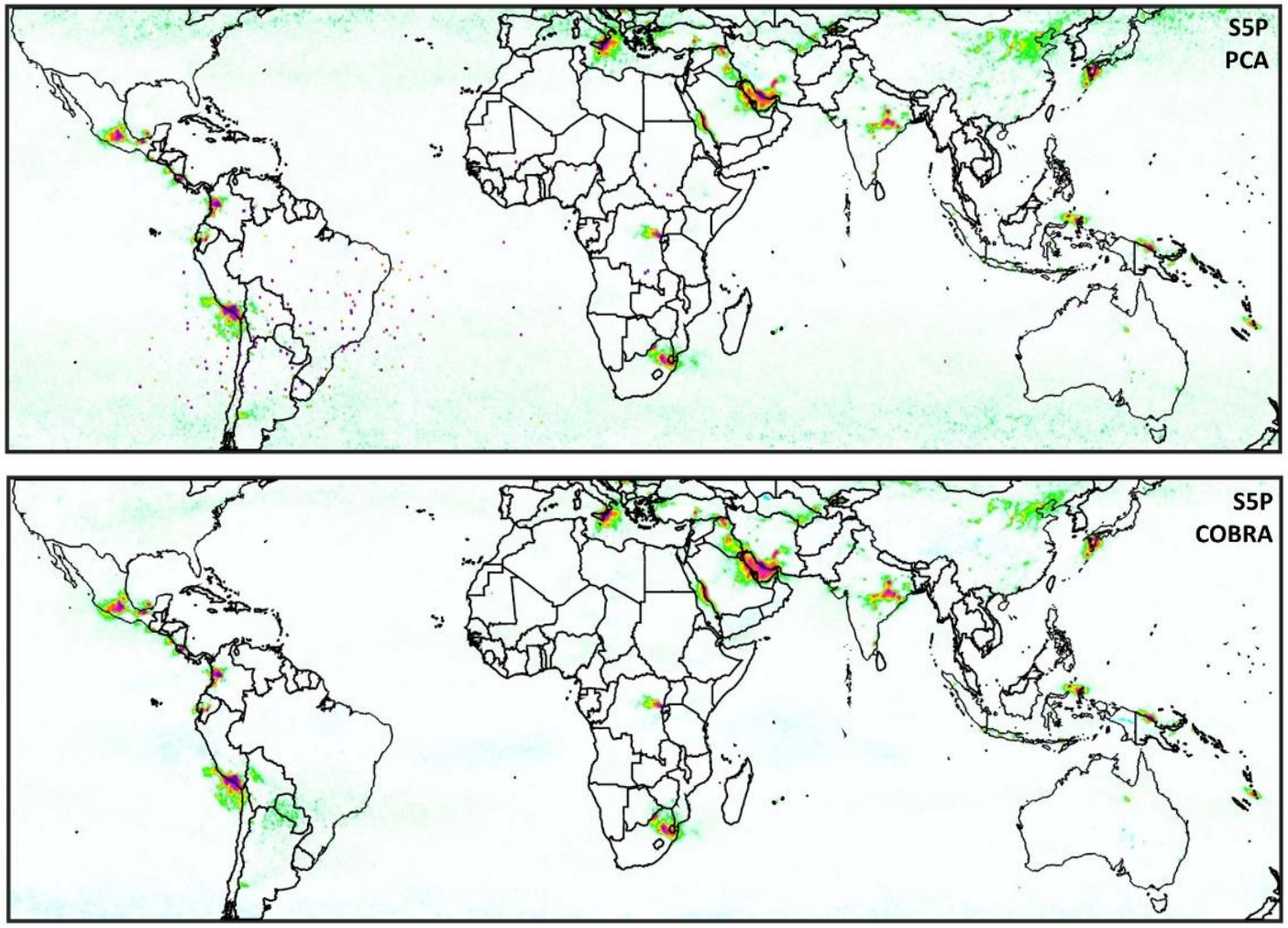

SO_2 VCD (DU)
09.2019-11.2019

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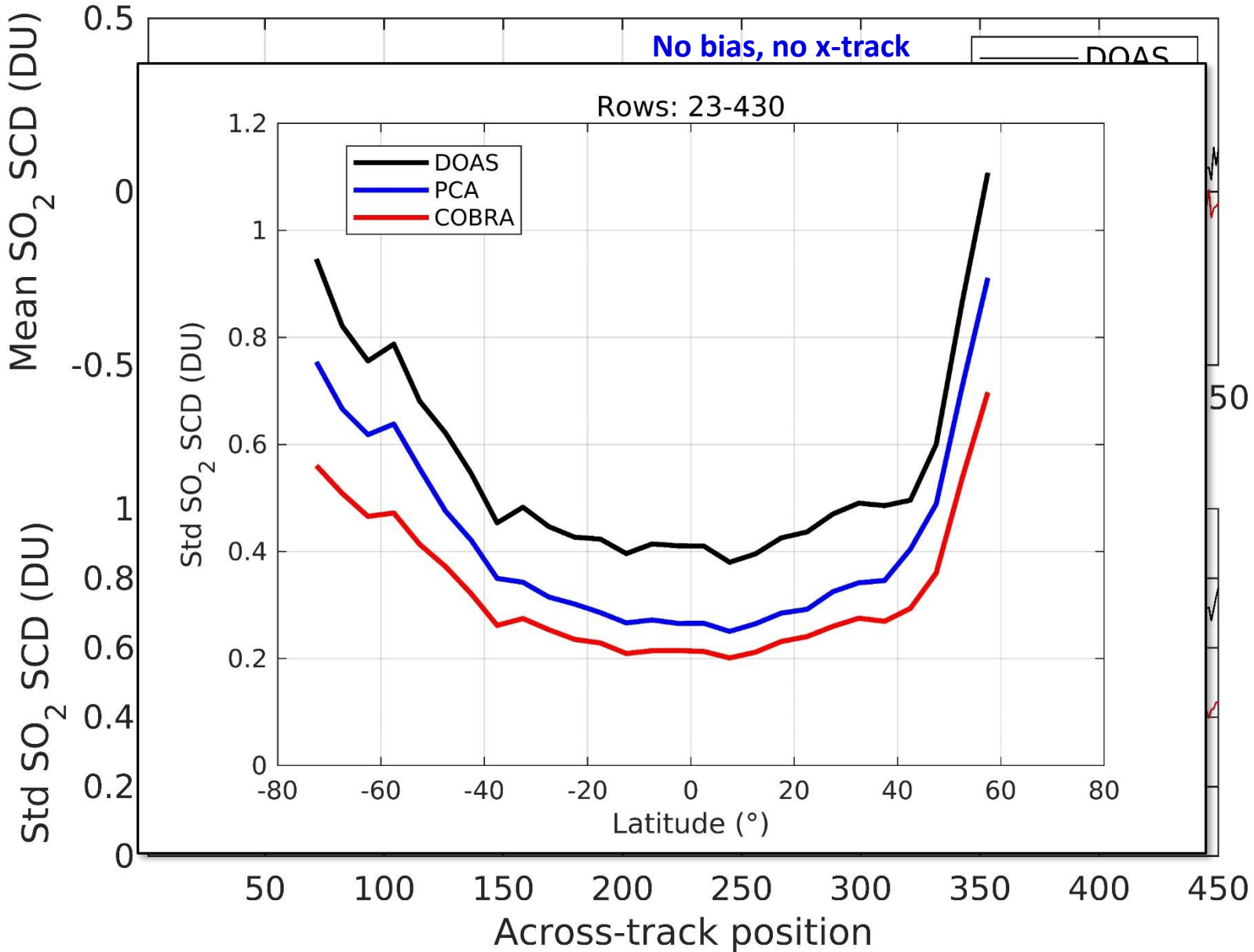
Bias and noise reduction



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Comparison with MAX-DOAS data

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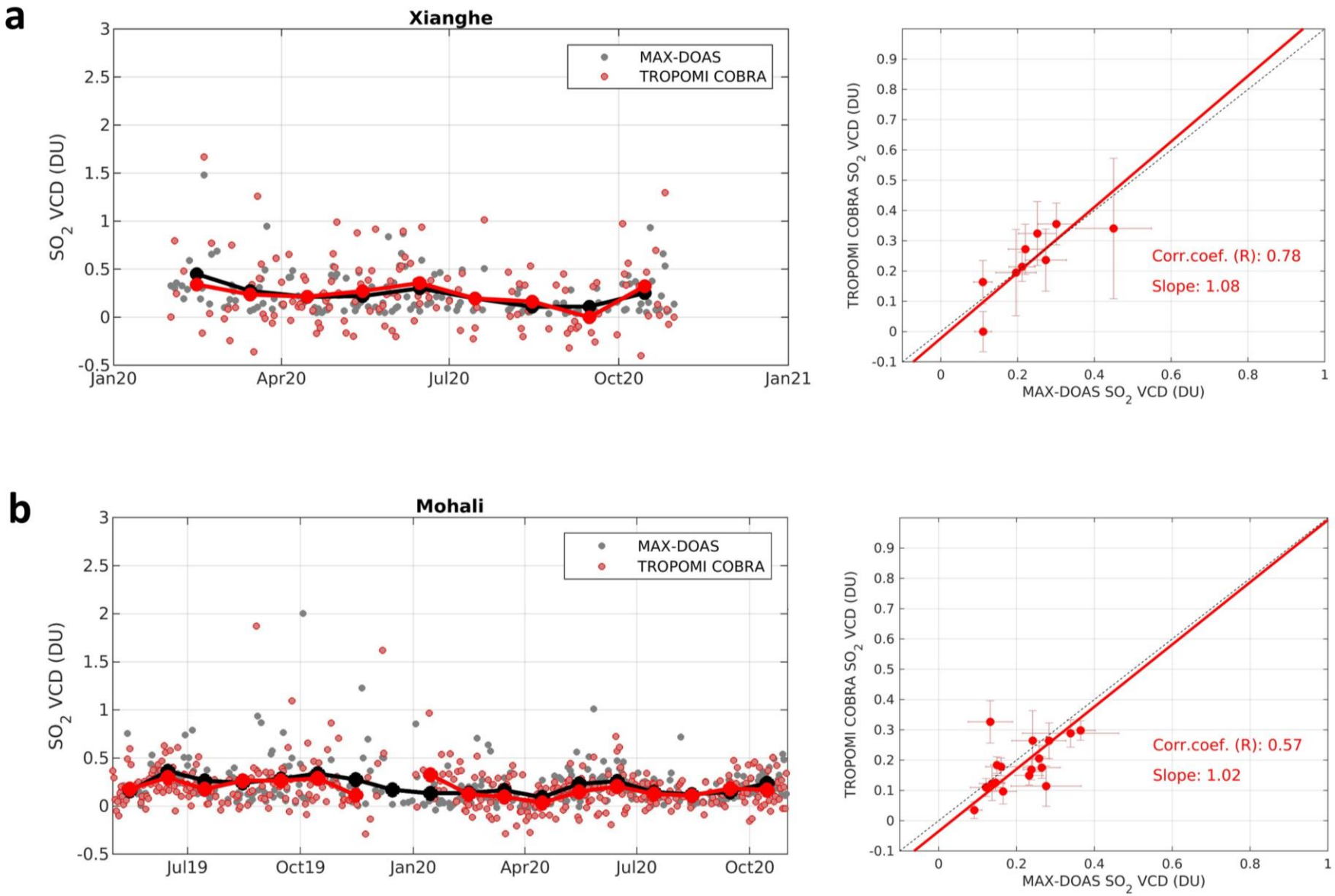

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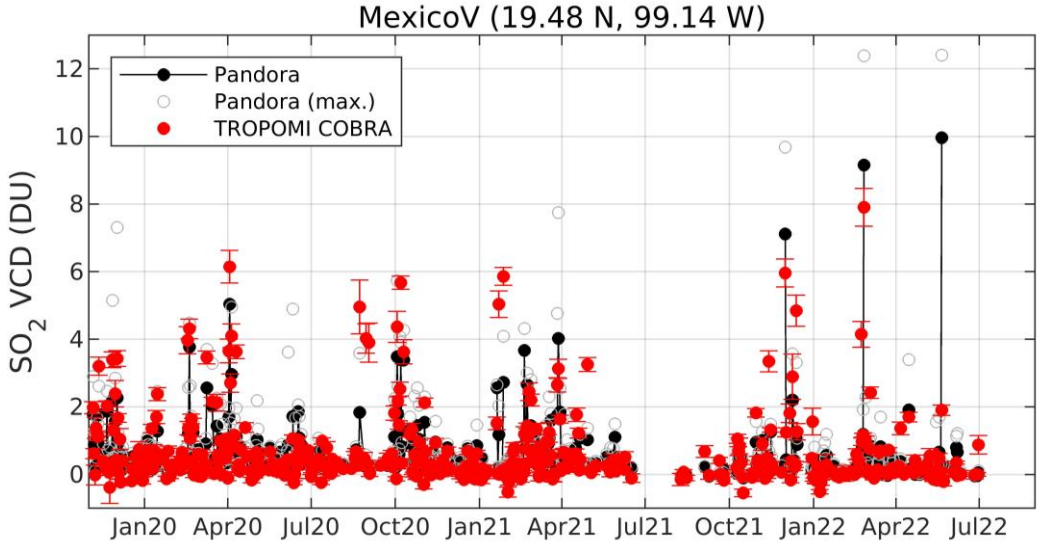
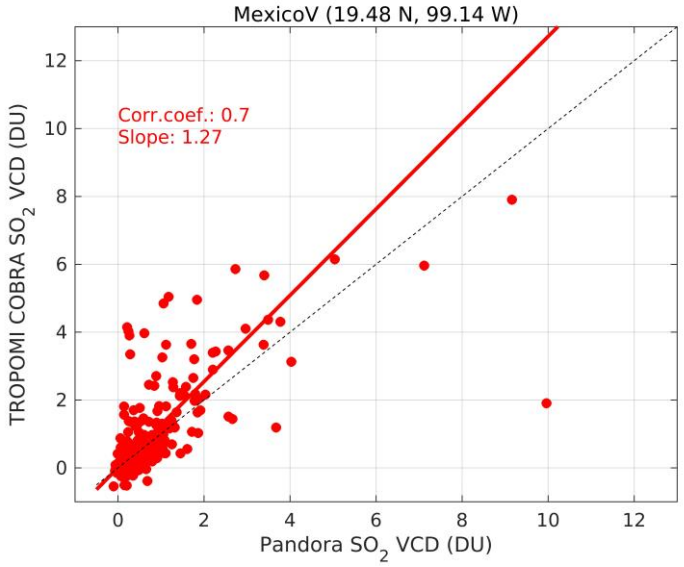
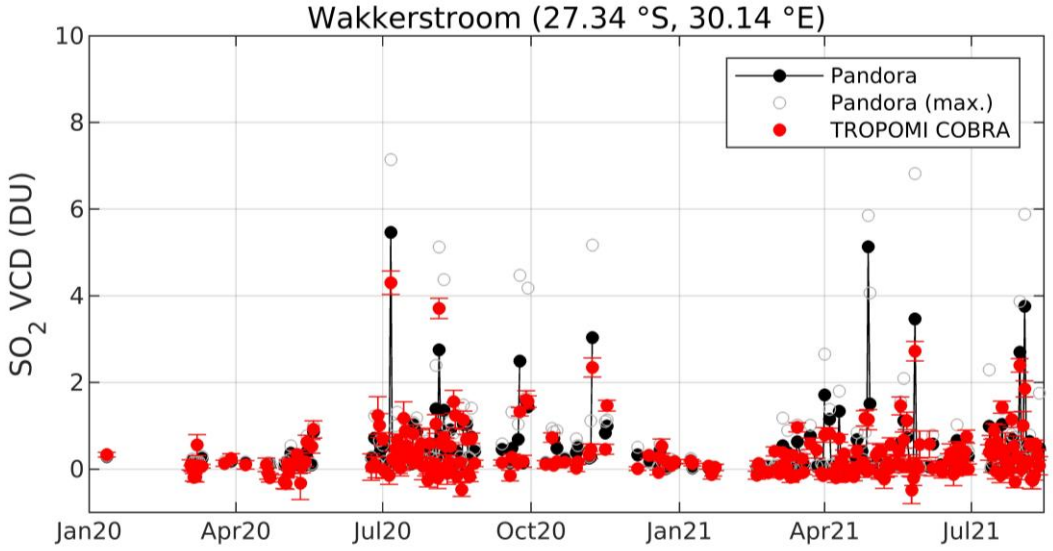
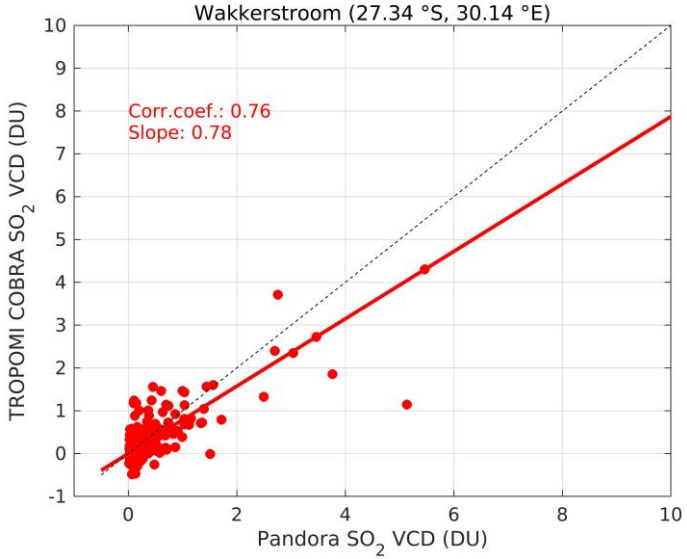
Comparison with Pandora data









Courtesy: A. Cede and M. Tiefengraber

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Long-term averages

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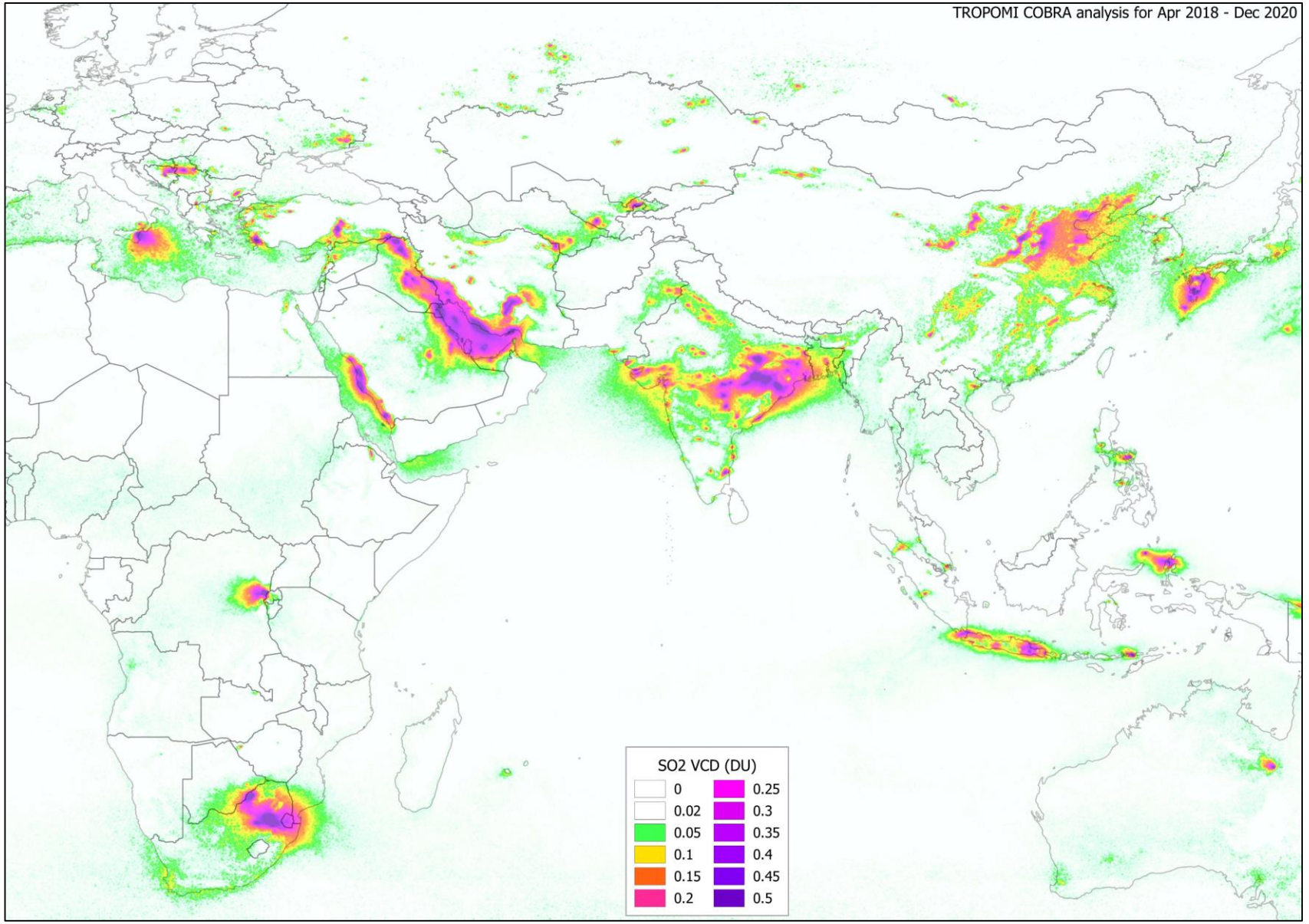

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Long-term averages

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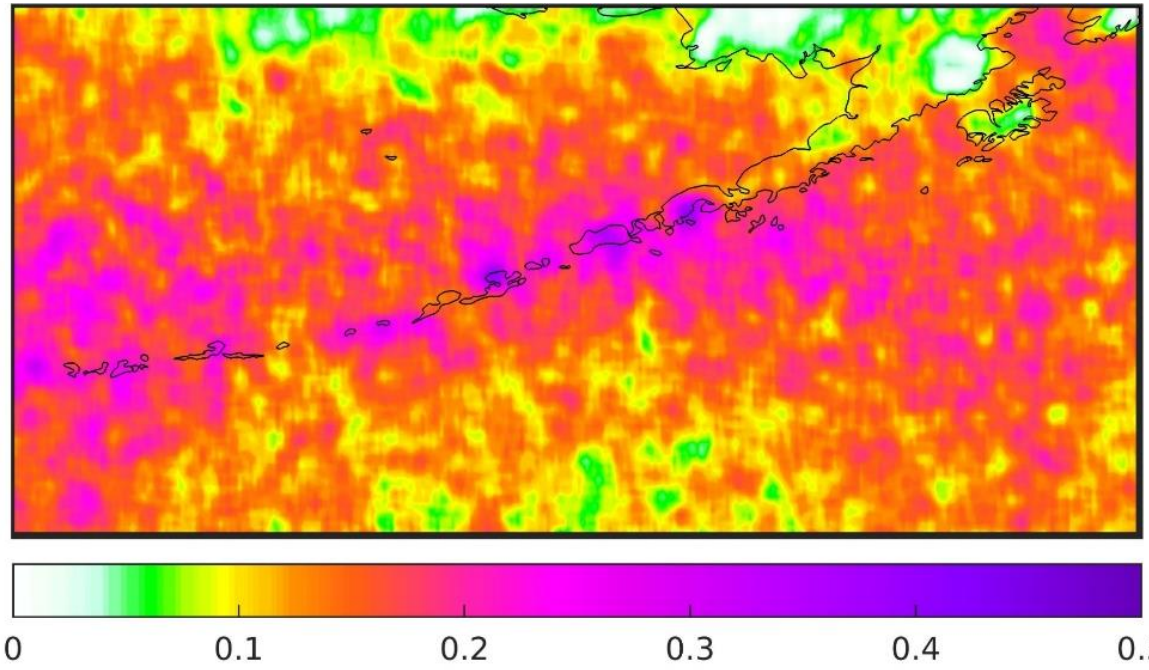
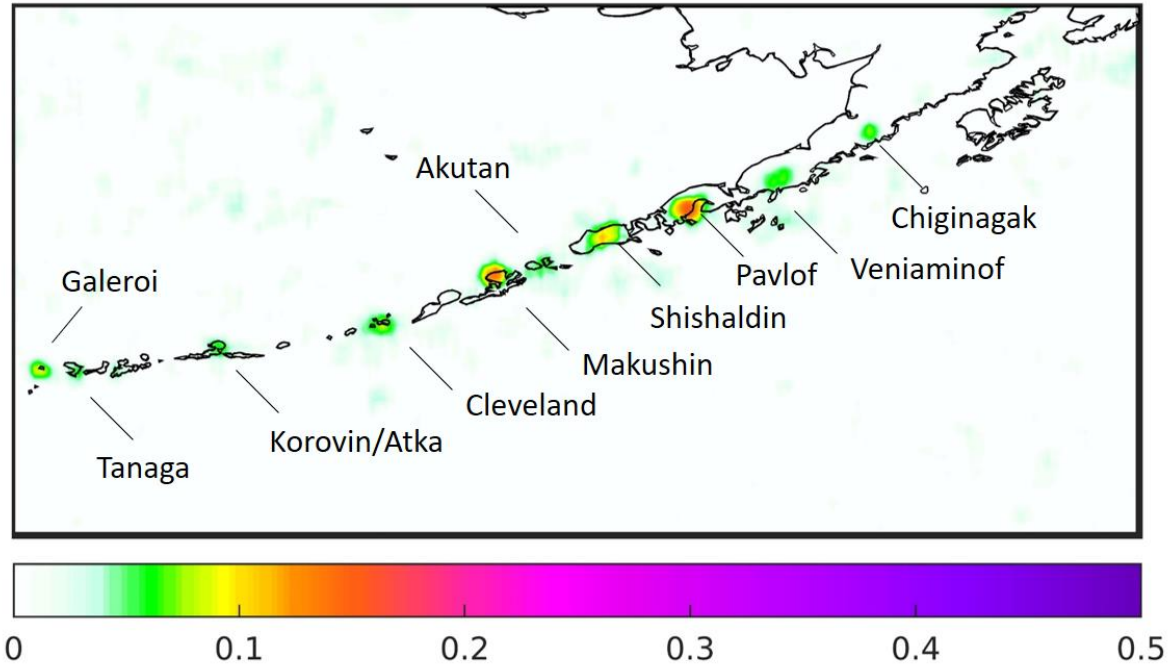
Aleutian Islands (Alaska) 05.2018-05.2020

Oper. product



COBRA



SO_2 VCD (DU)

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Long-term averages

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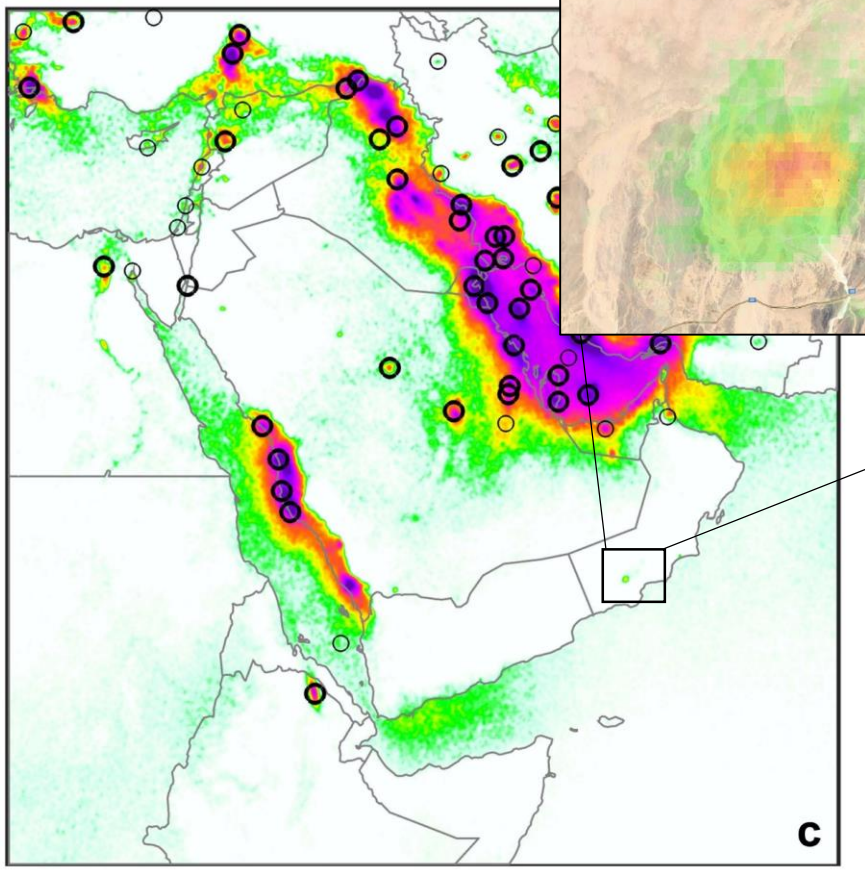
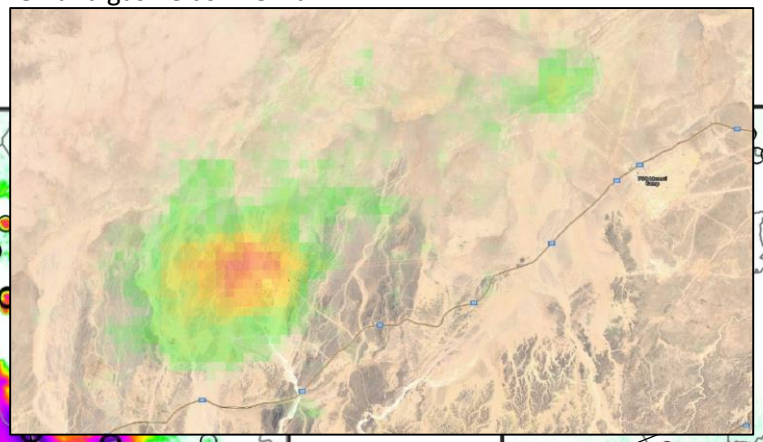
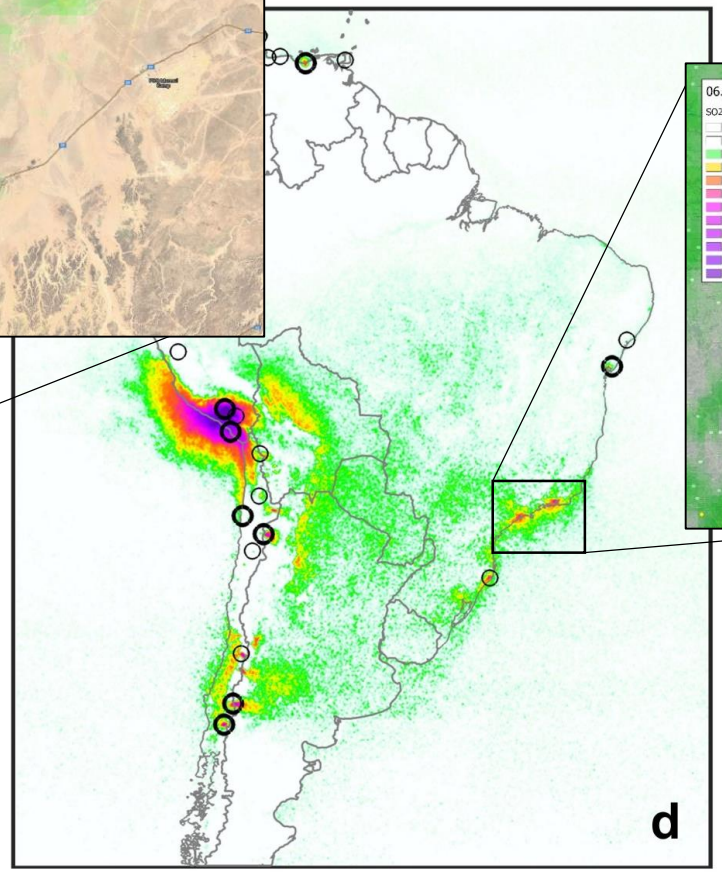
COBRA reveals new emission SO_2 sources

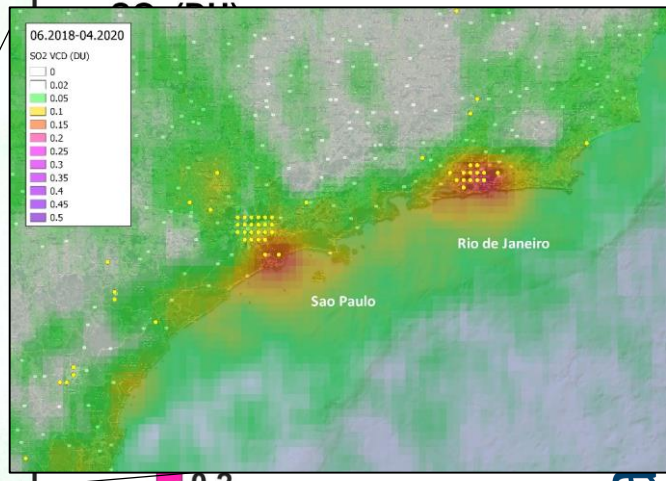
SO_2 sources detected by OMI

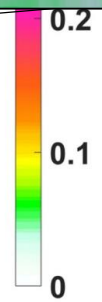
Oil and gas fields in Oman











SO_2 emissions estimates: 2005-2021

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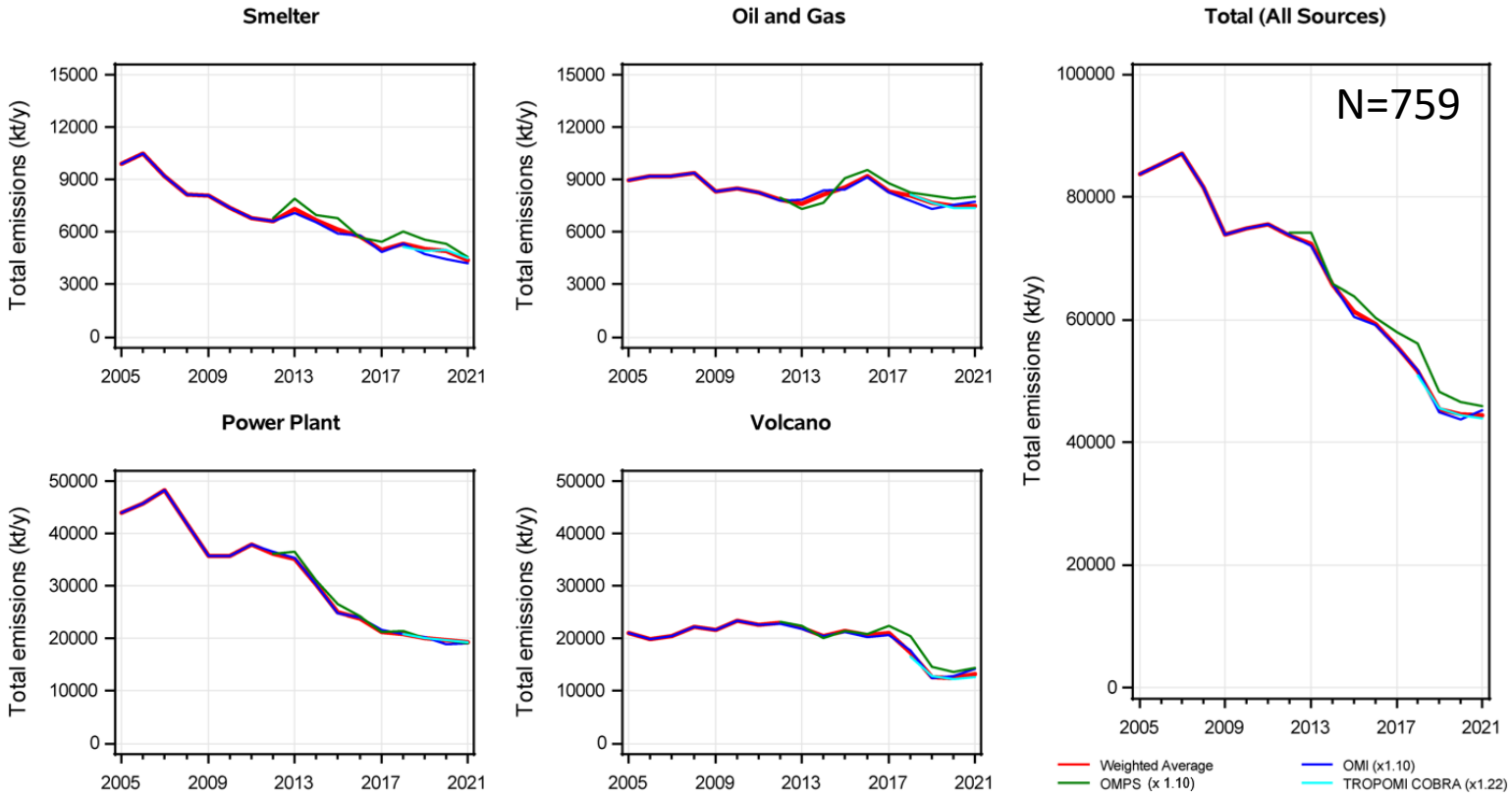
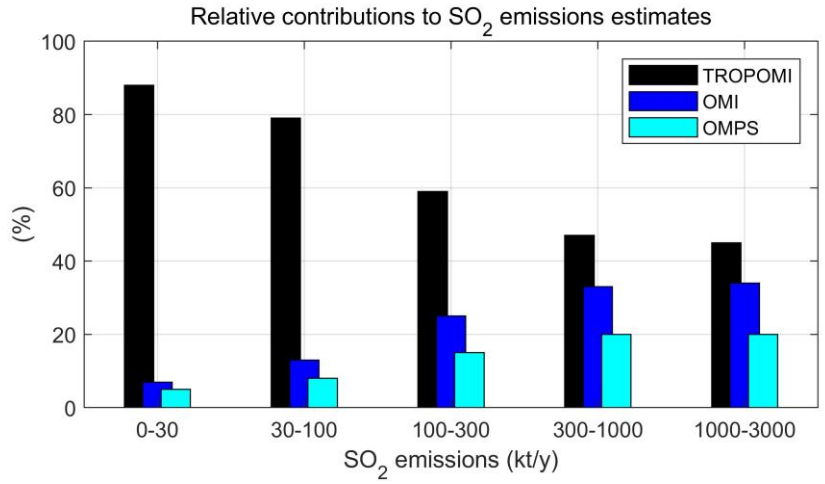
Global catalogue (v2) of SO_2 sources (see poster of V. Fioletov)





Adapted from Fioletov, et al. (Earth Syst. Sci. Data Discuss., in review).

https://so2.gsfc.nasa.gov/measures.html

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Extension of COBRA: SO_2 height

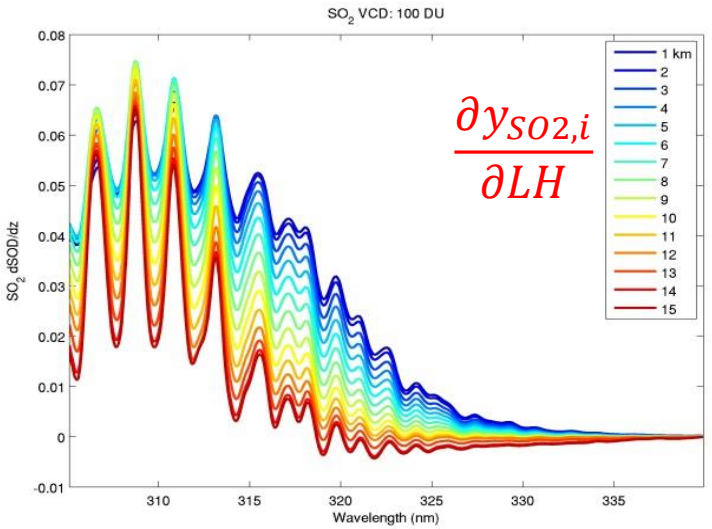
Extension of COBRA: SO_2 height

$$y = y_{SO2} + y_{bckg} + \epsilon$$

non-linear function of VCD and layer height (for high SO_2 loadings)
=> iterative approach

$$y_{SO2} = y_{SO2,i} + \alpha \frac{\partial y_{SO2,i}}{\partial VC} + \beta \frac{\partial y_{SO2,i}}{\partial LH}$$

Look-up-table of SO_2 spectra



$$\hat{x}_{i+1} = \hat{x}_i + \left(k_i^T S^{-1} k_i\right)^{-1} k_i^T S^{-1} (y_{meas} - y_{SO2,i} - \bar{y})$$

Theys et al., AMT, 2022

$x = \begin{bmatrix} LH \\ VC \end{bmatrix}$ SO_2 layer height and SO_2 column

$k_i = \begin{bmatrix} \frac{\partial y_{SO2,i}}{\partial LH} & \frac{\partial y_{SO2,i}}{\partial VC} \end{bmatrix}$ SO_2 Jacobeans

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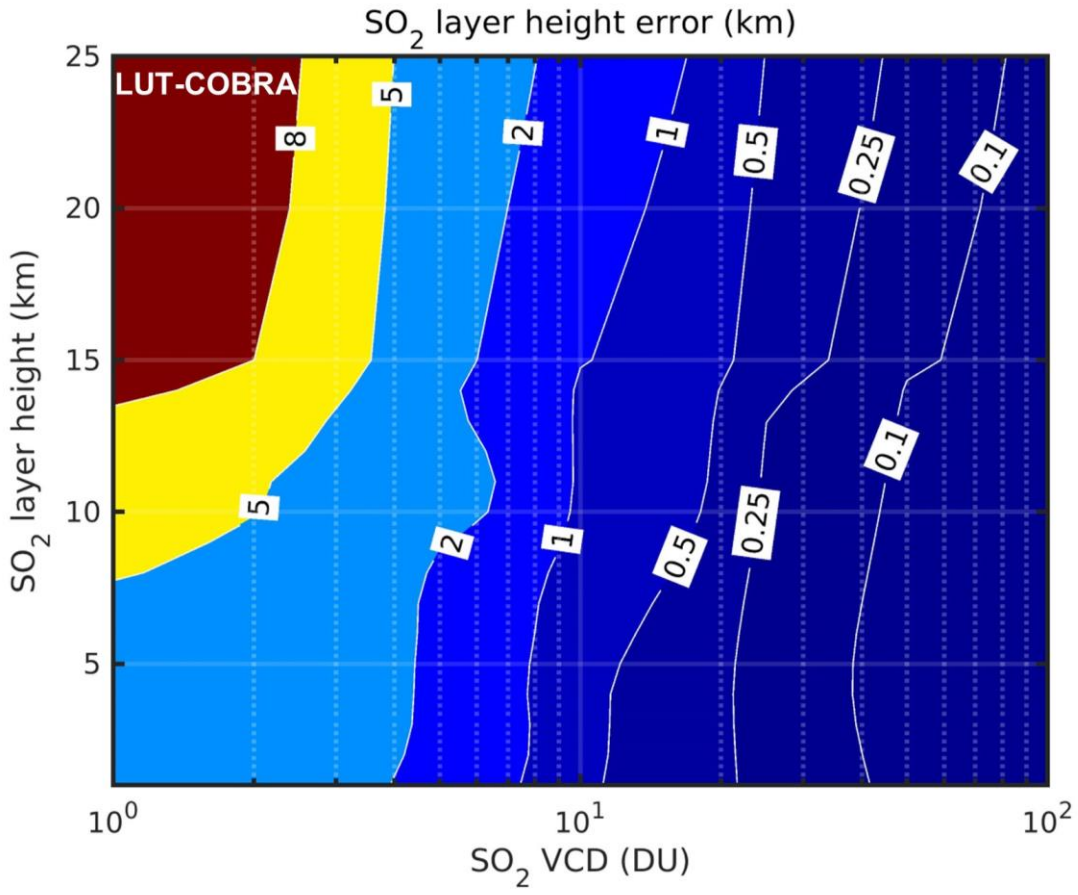
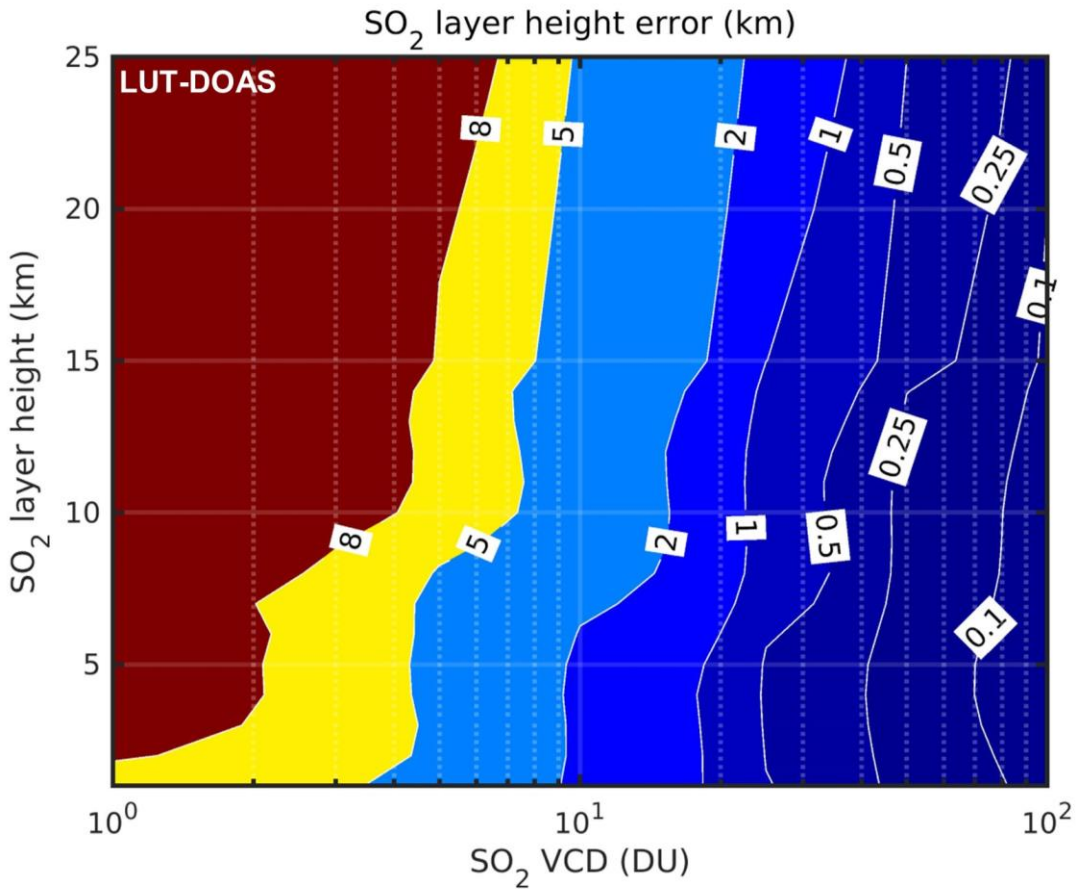
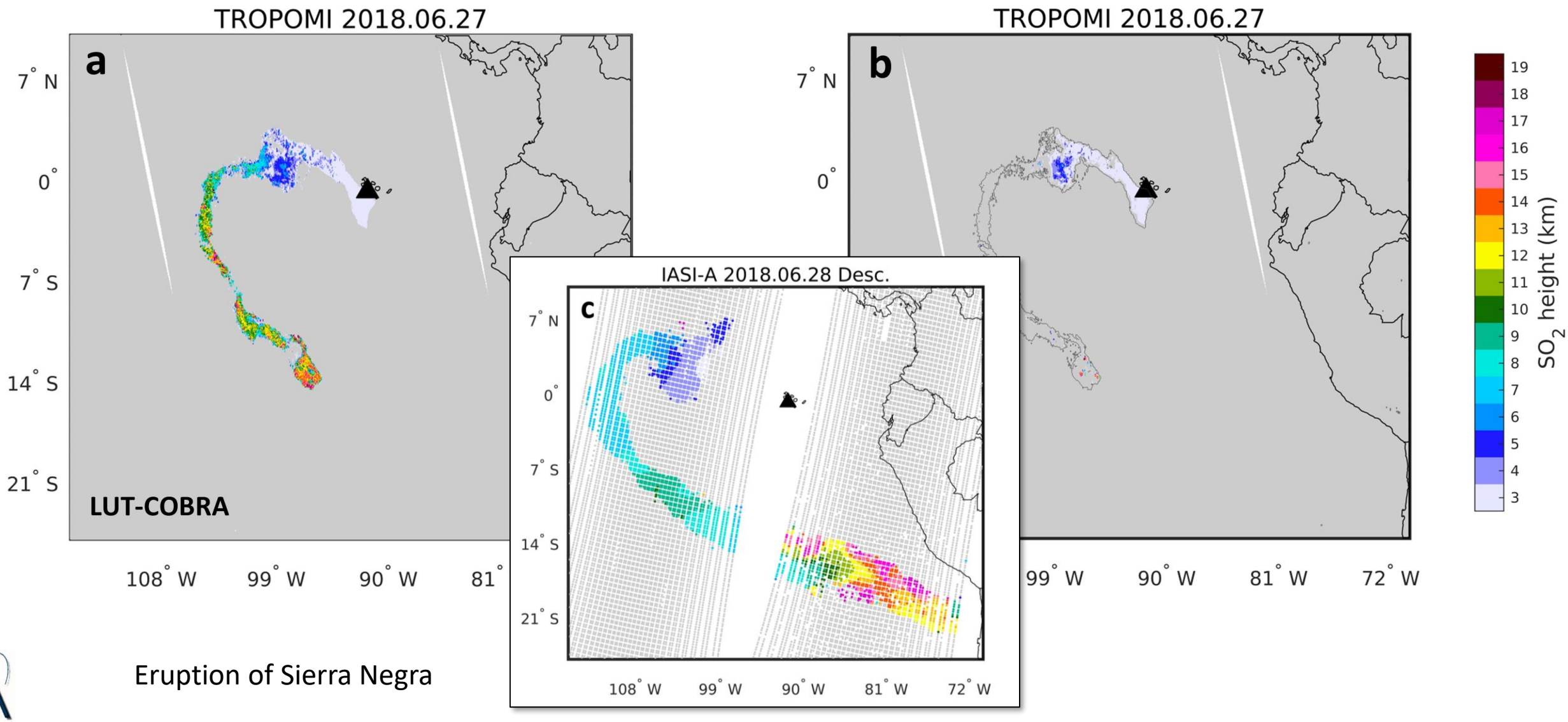
Gain in sensitivity





Gain in sensitivity



Eruption of Sierra Negra

Temporal analysis over degassing volcanoes

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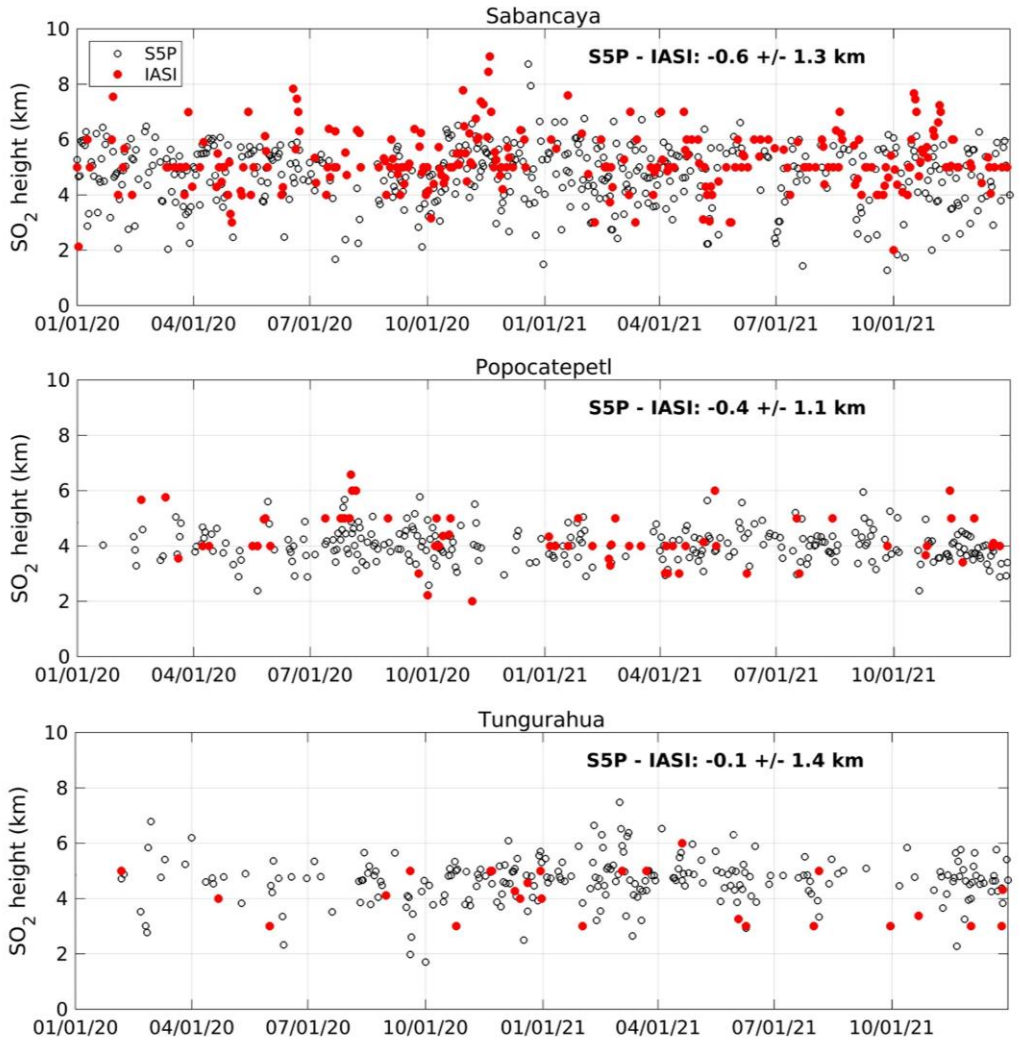

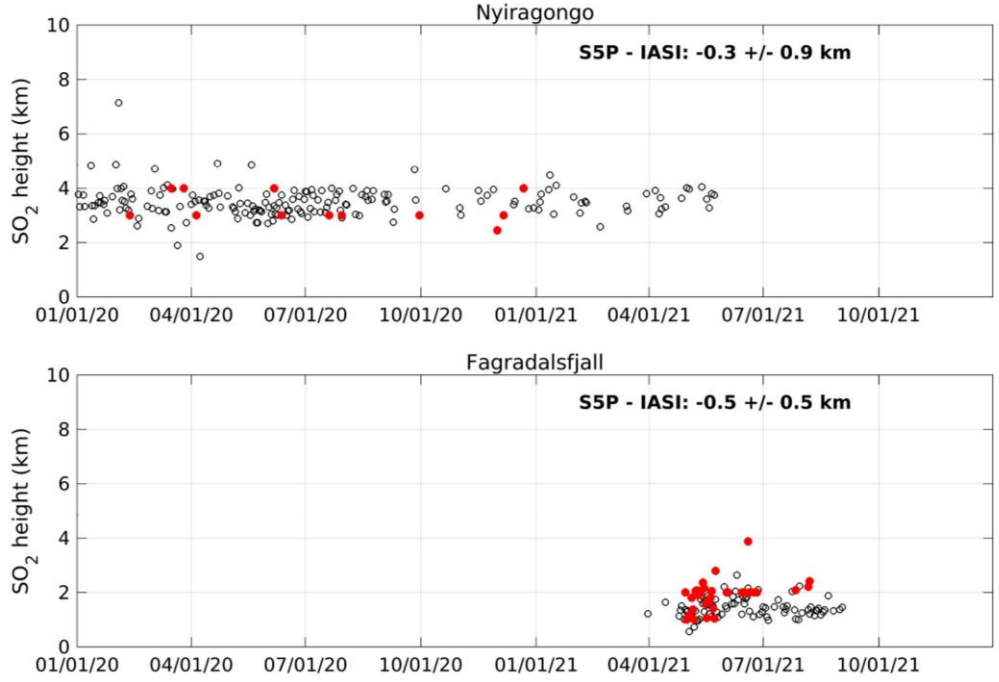

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Summary

- COBRA SO_2 VCD algorithm → **<u>improvement in sensitivity</u>**
  Reduction of bias and data scatter allows the study of weak SO_2 sources.

- Good comparison between S5P COBRA and S5P PCA.
  Encouraging comparison with MAXDOAS and Pandora instruments.

- COBRA improves the limit of detection for SO_2 emissions as low as ~8 kt SO_2/year.

- Extension of COBRA for the retrieval of SO_2 height, using an iterative look-up-table approach. Sensitivity down to 5 DU.

- COBRA is a promising approach not only for Sentinel-5 Precursor but also for geostationary sensors like Sentinel-4.

Product availability and next steps

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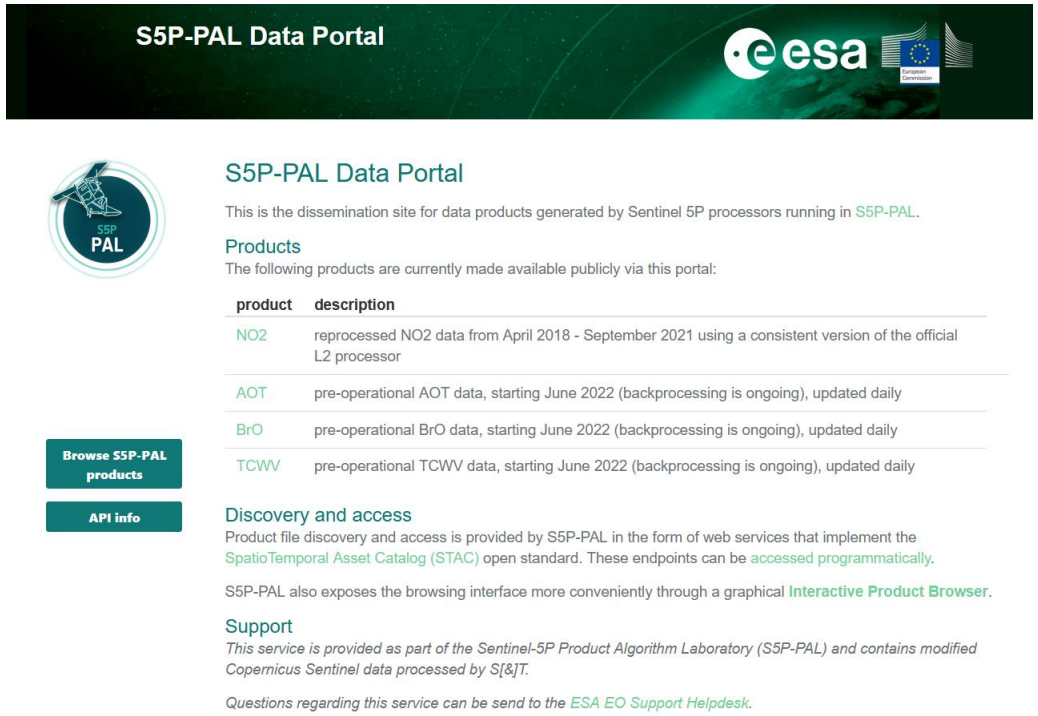
- S5P_PAL__L2__SO2CBR_ soon in PAL (same format as operational product).
- Further development and refinement of the algorithm in the next months (v2).
- Implementation in operational environment (end 2023).



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Perspectives: long-term data record

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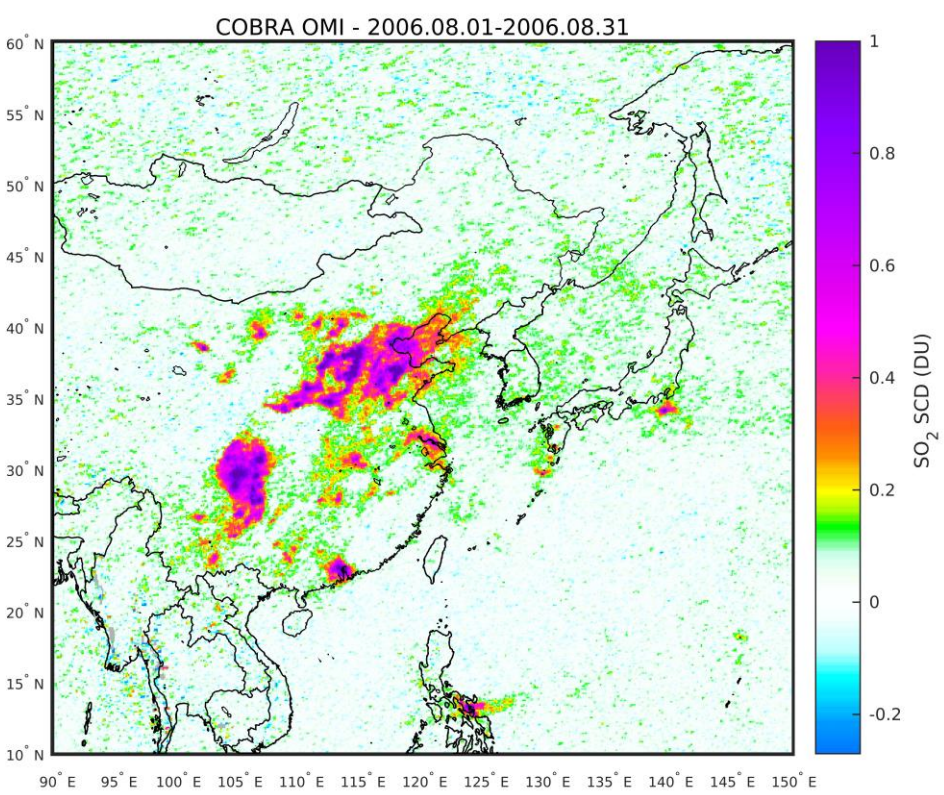
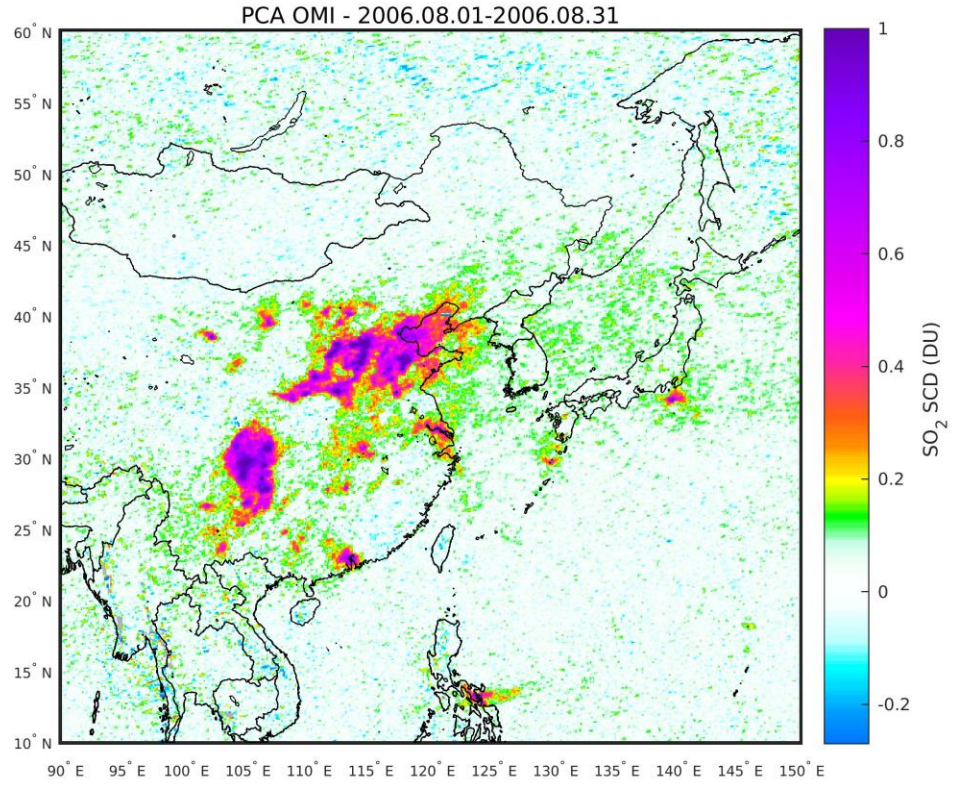
Generation of multi-decadal SO_2 data set using COBRA from GOME-1, SCIAMACHY, OMI and TROPOMI

Climate Change Initiative
Precursors for aerosols and ozone

precursors cci

preliminary





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