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### Advanced retrieval of SO<sub>2</sub> from TROPOMI using COBRA

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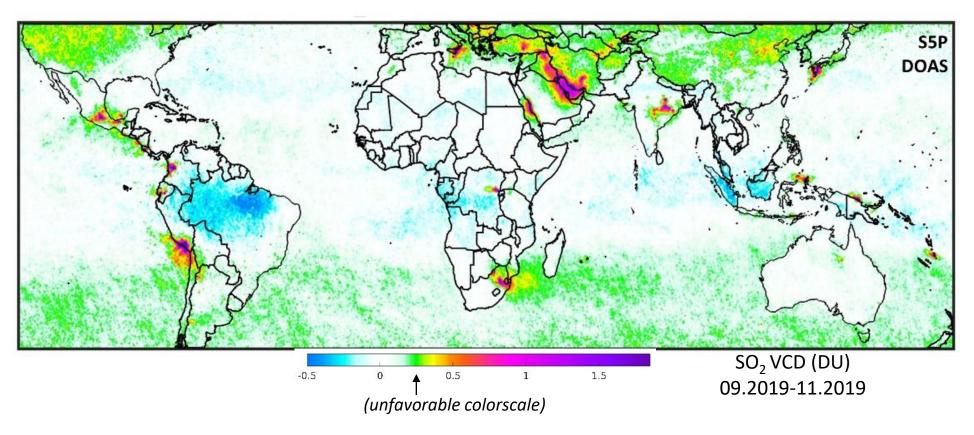


#### Motivation

Weak emission sources are difficult to study with current TROPOMI SO<sub>2</sub> product because of large scale biases (~0.2 DU), in part due to imperfect Ring correction.

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=> 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
\vec{\epsilon}: measurement error

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

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

**Note:** most often,  $S_{\in}$  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<sub>2</sub>.  $y_{bck}$ : -log(I/Io) without contribution from SO<sub>2</sub>

$$\rightarrow \widehat{SCD} = (k^T S^{-1} k)^{-1} \cdot k^T S^{-1} \cdot (y - \overline{y})$$

**Assumption:**  $y_{bck} + \epsilon$  can be considered as an error term, characterized by a mean spectrum  $\overline{y}$  and an error covariance matrix  $S(pdf Gaussian distribution) => S and <math>\overline{y}$  are obtained from a set of SO<sub>2</sub>-free <u>measured</u> spectra

Implementation (Theys et al., ACP, 2021)

- S (and  $\overline{y}$ ) 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

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



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

#### TROPOMI SO<sub>2</sub> products comparison

-0.5

0.5

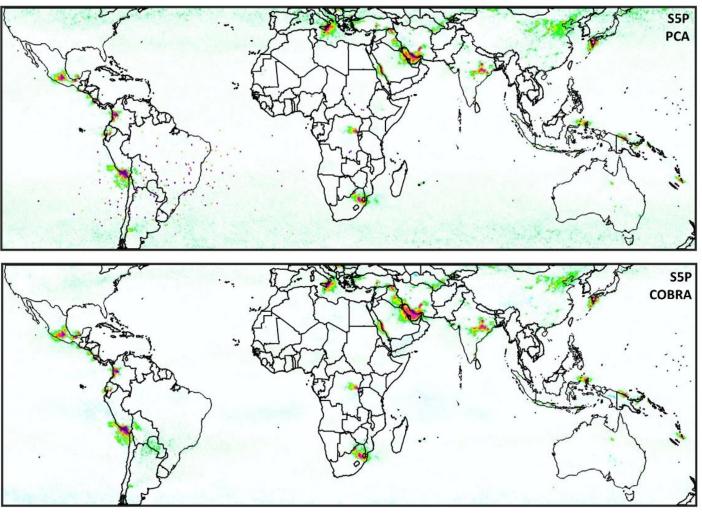
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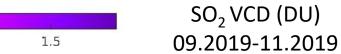
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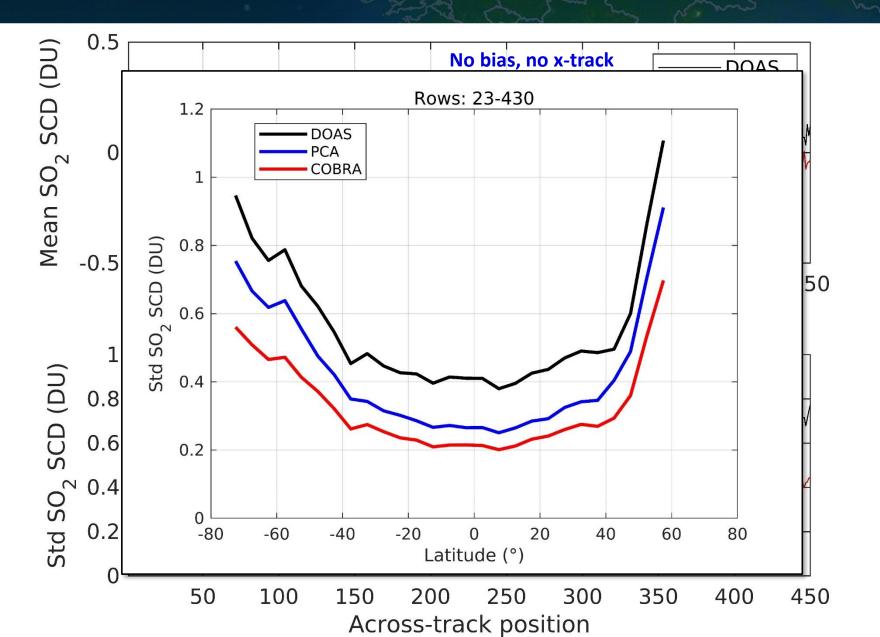








#### Bias and noise reduction



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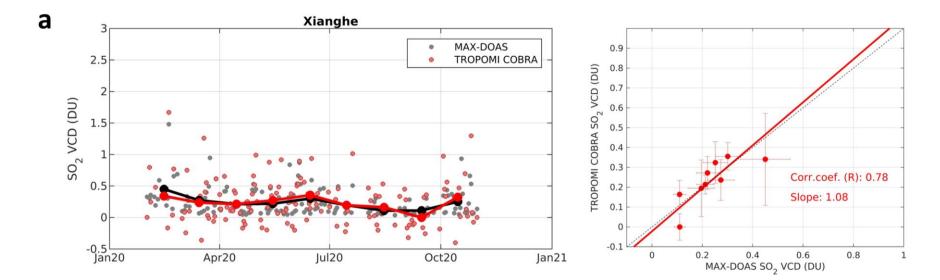
#### Comparison with MAX-DOAS data

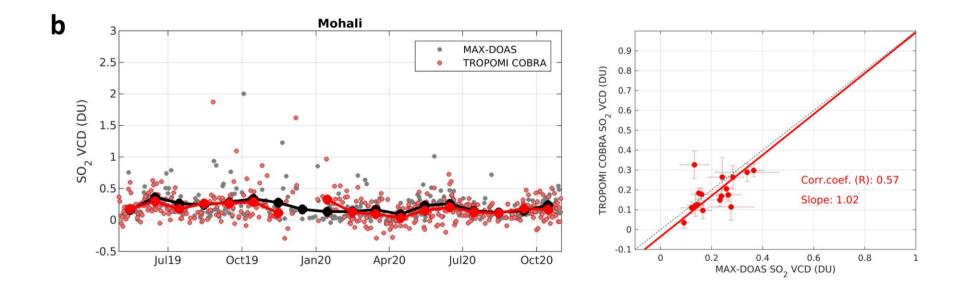
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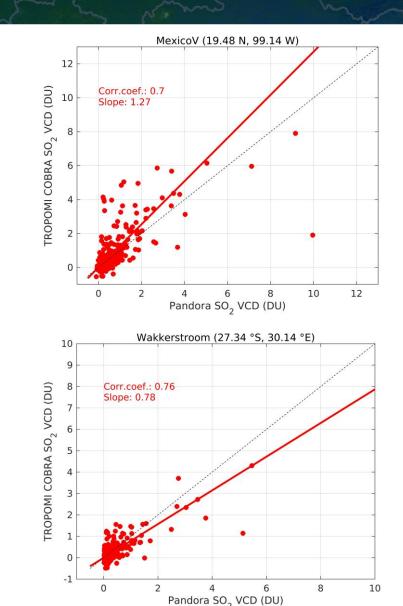


#### Comparison with Pandora data

Jan20 Apr20 Jul20 Oct20 Jan21 Apr21 Jul21 Oct21 Jan22 Apr22 Jul22

Wakkerstroom (27.34 °S, 30.14 °E) 10 Pandora Pandora (max.) 8 **TROPOMI COBRA** VCD (DU) SO<sub>2</sub> 0 Jan20 Apr20 Jul20 Oct20 Jan21 Apr21 Jul21

Courtesy: A. Cede and M. Tiefengraber



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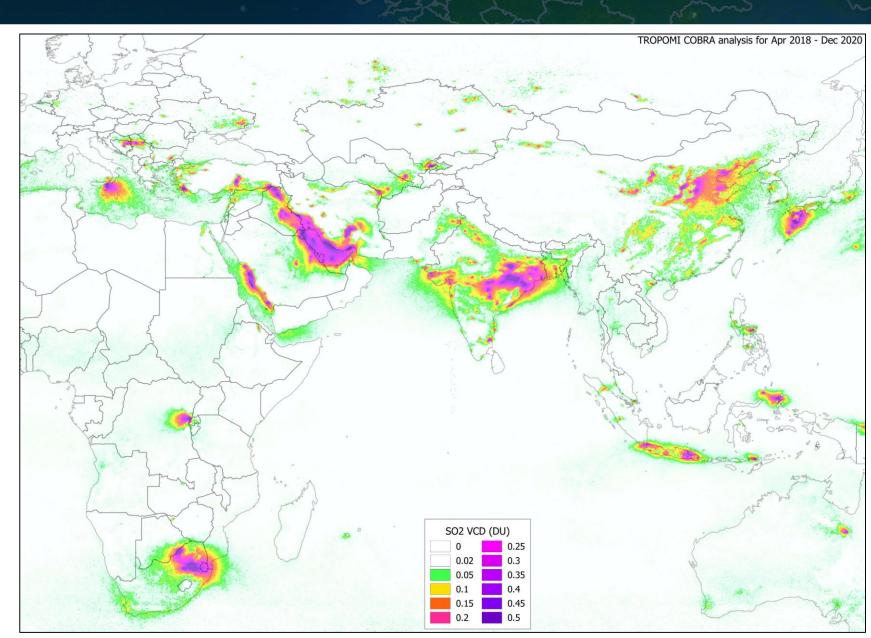
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#### Long-term averages

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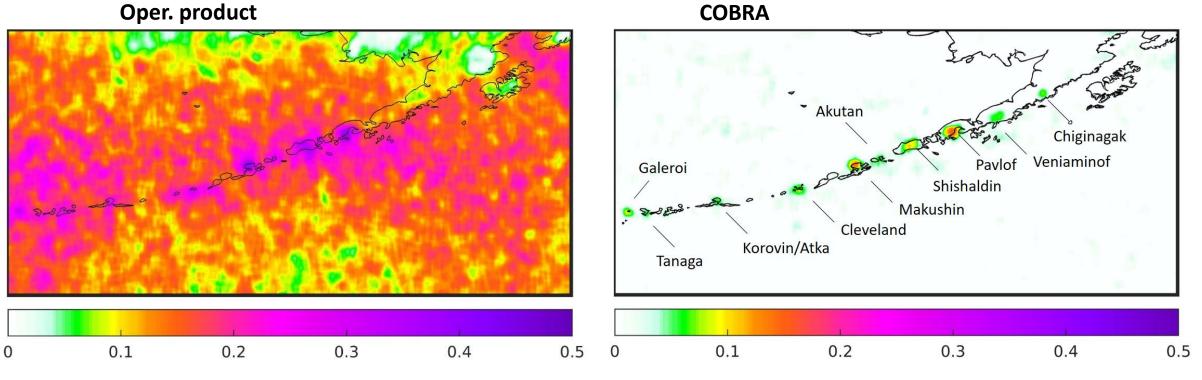
#### Long-term averages

Aleutian Islands (Alaska) 05.2018-05.2020

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#### **Oper. product**



 $SO_2$  VCD (DU)

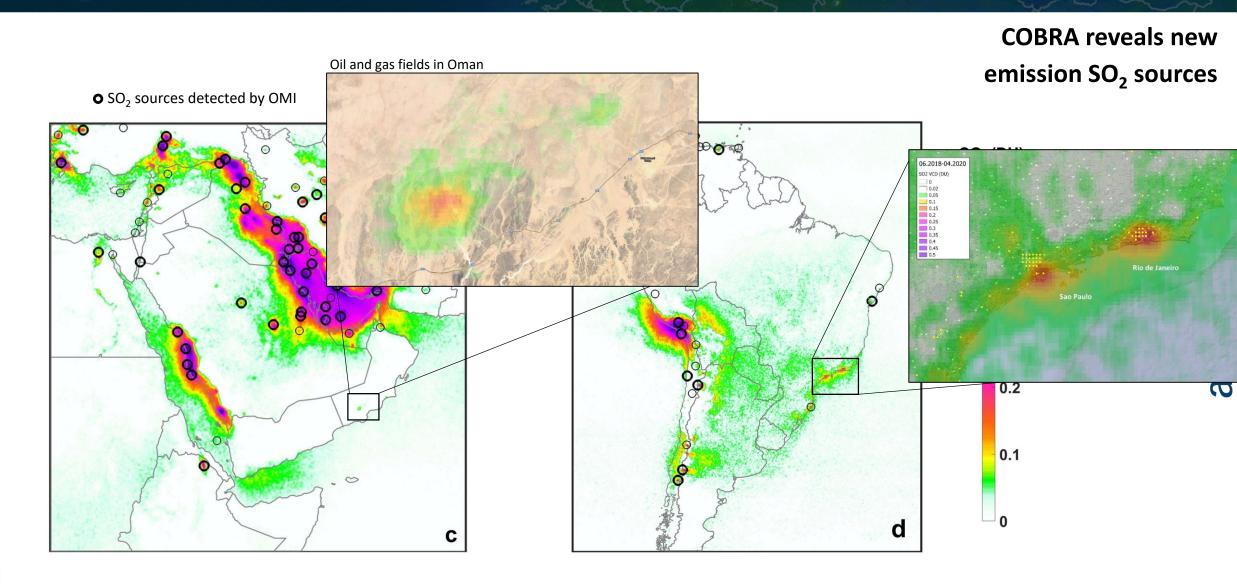
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#### Long-term averages



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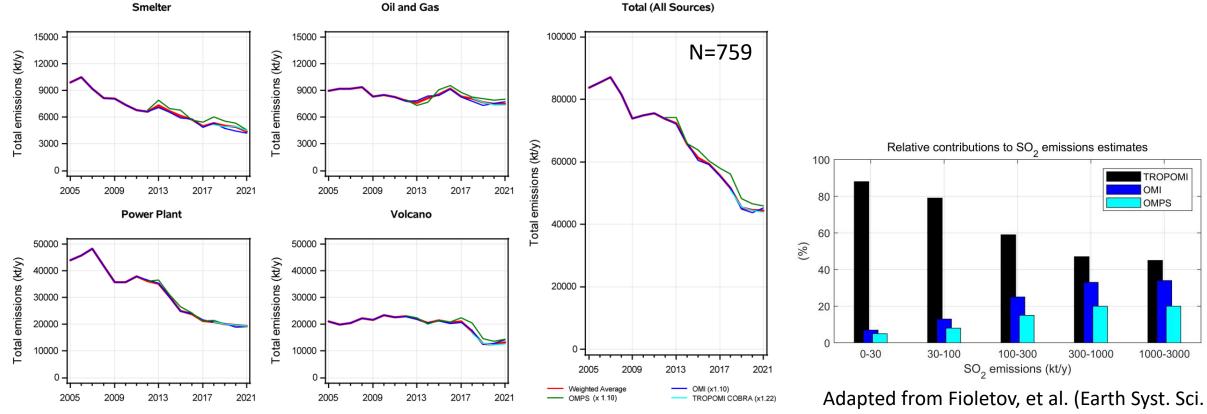
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#### Global catalogue (v2) of SO<sub>2</sub> sources (see poster of V. Fioletov)



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



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Data Discuss., in review).



### Extension of COBRA: SO<sub>2</sub> height



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

non-linear function of VCD and layer height (for high SO<sub>2</sub> loadings) => iterative approach

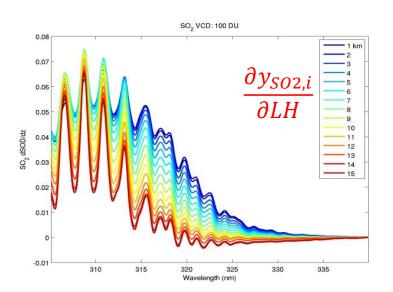
$$\Rightarrow y_{SO2} = y_{SO2,i} + \alpha \frac{\partial y_{SO2,i}}{\partial VC} + \beta \frac{\partial y_{SO2,i}}{\partial LH}$$
Look-up-table of SO<sub>2</sub> spectra

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

Theys et al., AMT, 2022

$$x = \begin{bmatrix} LH \\ VC \end{bmatrix}$$
 SO<sub>2</sub> layer height and SO<sub>2</sub> column

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



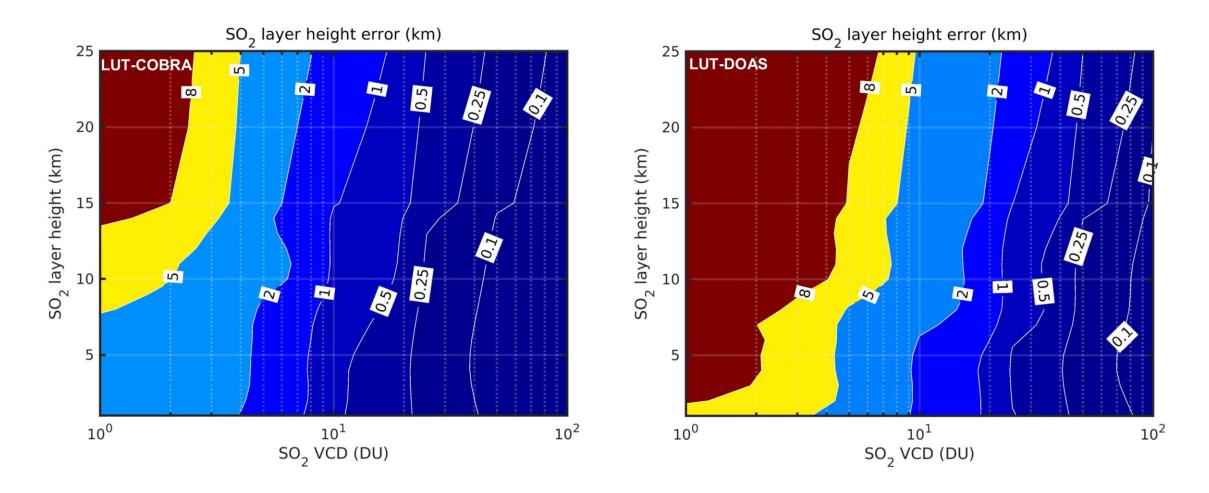
#### Gain in sensitivity

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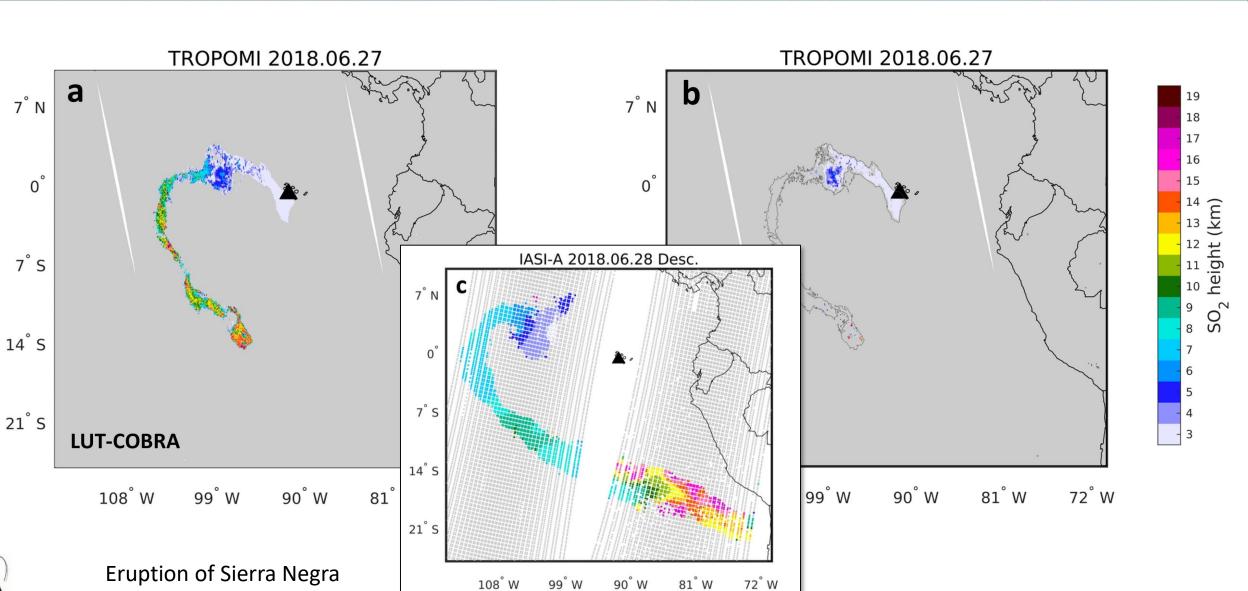
#### Gain in sensitivity



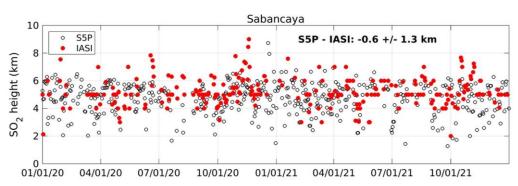
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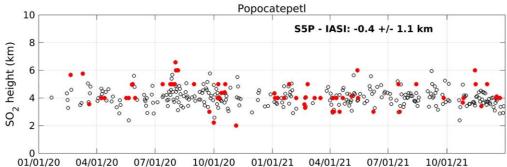
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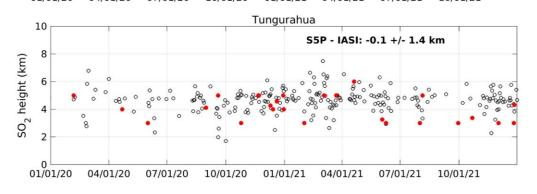
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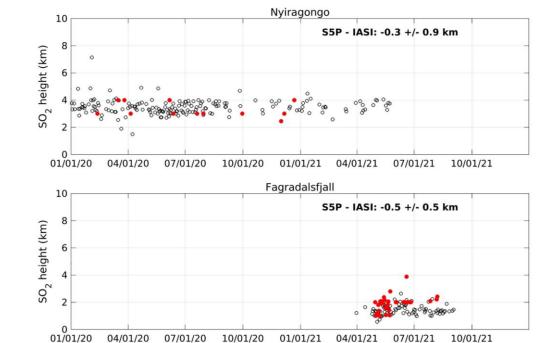


### Temporal analysis over degassing volcanoes









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- COBRA SO<sub>2</sub> VCD algorithm → <u>improvement in sensitivity</u> Reduction of bias and data scatter allows the study of weak SO<sub>2</sub> 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<sub>2</sub> 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.

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#### Product availability and next steps

- 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).

S5P-	PAL Data	a Portal
		AL Data Portal
	Products	dissemination site for data products generated by Sentinel 5P processors running in S5P-PAL. Ing products are currently made available publicly via this portal:
	product	description
	NO2	reprocessed NO2 data from April 2018 - September 2021 using a consistent version of the official L2 processor
	AOT	pre-operational AOT data, starting June 2022 (backprocessing is ongoing), updated daily
	BrO	pre-operational BrO data, starting June 2022 (backprocessing is ongoing), updated daily
	TCWV	pre-operational TCWV data, starting June 2022 (backprocessing is ongoing), updated daily
	Discovery and access Product file discovery and access is provided by S5P-PAL in the form of web services that implement the SpatioTemporal Asset Catalog (STAC) open standard. These endpoints can be accessed programmatically.	
	S5P-PAL also exposes the browsing interface more conveniently through a graphical Interactive Product Browse	
	Support This service is provided as part of the Sentinel-5P Product Algorithm Laboratory (S5P-PAL) and contains modified Copernicus Sentinel data processed by S[&]T.	
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Questions regarding this service can be send to the ESA EO Support Helpdesk.

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#### Perspectives: long-term data record

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0.8

0.6

0.4

0.2

- 0

-0.2

SCD (DU)

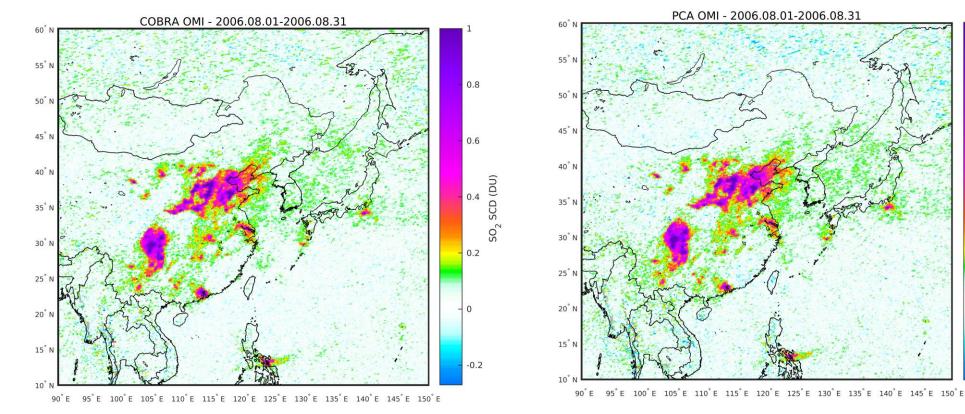
SO.

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Generation of multi-decadal SO<sub>2</sub> data set using COBRA from GOME-1, SCIAMACHY, OMI and TROPOMI

*Climate Change Initiative Precursors for aerosols and ozone* 





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### Thank you for your attention!