Enhancing global SO₂ emission inventories using S5P/ **TROPOMI** satellite measurements

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1. Motivation

- sulfur dioxide (SO₂) is a major air pollutant
- · affects atmospheric chemistry, environment, climate, and human health
- SO₂ emission sources: • anthropogenic: coal-burning, power plants, oil refineries, and
 - smelters
 - natural: volcanic eruptions, volcanic degassing, and wildfires
- accurate information about SO₂ emissions is required in air quality and climate models

Aims of this study

- identification of anthropogenic SO₂ sources and derivation of a global emission inventory
- · comparison of derived emissions with existing emission catalogues
- investigation to other species (e.g. NO_x)
- optimization of emission estimations using new algorithms & methods

2. Algorithm

1. Data selection

- COBRA SO₂: decreases noise and biases significantly
- ERA5 winds: ECMWF atmospheric reanalysis of the global climate
- 2. Data filtering & merging
 - restriction to QA values above 0.5
 - removal of artifacts due to COBRA algorithm
 - merging of COBRA and DOAS SO₂ datasets
- 3. AMF correction
- based on averaging kernel at plume altitude to account for height dependent sensitivity 4. Derivative on TROPOMI grid
 - interpolation of wind fields to 500 m, obs. time and lat/lon of TROPOMI pixel center
 - calculation of gradient of the SO₂ VCD on TROPOMI grid (as proposed by de Foy, 2022)
- 5. Calculation of advection
- see section 3
- 6. Topographic correction
 - systematic artifacts of the divergence map over mountains
 - calculation of topography-corrected advection to account for 3D transport effects (according to Sun, 2023)
- 7. Gridding and averaging
 - re-gridding to a regular lat/lon grid with 0.025° resolution
 - temporal averages for daily, monthly, and annual periods + complete time series
- 8. Compilation of point source (ps) catalogue
 - 1. ps are identified by a fully automated iterative procedure
 - 2. ps are quantified by spatial integration of the advection map
 - 3. significant ps are selected by different criteria (e.g. temporal persistence)

3. Advection method

• starting point: divergence of SO₂ flux based on continuity equation

$$\bullet D = \nabla \cdot F = E - F$$

 $\bullet D = \nabla \cdot (\overrightarrow{w}V) = \overrightarrow{w} \cdot \nabla V + V \nabla \cdot \overrightarrow{w}$

- first term is the advection of SO₂
 - $\cdot A = \overrightarrow{w} \cdot \nabla V$
- second term: divergence of the wind fields scaled with the SO₂ VCD
- we are interested in flux changes caused by local SO₂ emissions \Rightarrow advection method
- method yields sources/sinks on a map



4. Results (global)

- anthropogenic as well as volcanic sources are clearly visible in the total mean SO₂ map
- mostly small and medium emission sources are detected as point sources
- SO₂ sources with very high emission values are not yet classified correctly e.g. volcanoes and strong anthropogenic sources like Norilsk (Russia) • due to their spatial extent, some of the sources get classified as "area sources" (not listed yet)
- in case of complex topography or SO₂ sinks in proximity of the source, some SO₂ sources get classified as "negative" this phenomena is often observed near volcanoes



5. Results (regional)

- regions of enhanced SO₂ are already evident from the VCD maps
- · exact location is inferred from the advection method
- on local scale: very good agreement with NO_x point source catalogue
- background is much more noisy than for NO_x this makes the weak sources more difficult to distinguish from the background



- **REFERENCES:** 1. Beirle, Steffen, et al. "Pinpointing nitrogen oxide emissions from space." *Science advances* 5.11 (2019): eaax9800. 2. Beirle, Steffen, et al. "Improved catalog of NO_x point source emissions (version 2)." *Earth System Science Data Discussions* (2023): 1-37.

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- total number of anthropogenic sources is 200+

Outlook

- further comparison with existing SO₂ catalogues
- include external information about the source

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6. SO₂ point source catalogue extract (preliminary)

• in addition to emissions, statistics for the point sources will be provided

Top 10 anthropogenic emission sources (global)

ank	Latitude [°]	Longitude [°]	Emissions [kt/month]	Error [kt/month]
	-23.69	27.59	35.08	24.83
	-4.06	145.04	34.69	24.67
	17.89	-93.19	23.47	16.65
	31.59	130.66	17.74	12.68
	-26.26	29.16	17.67	12.68
	22.66	39.04	16.46	11.65
	38.36	36.99	16.38	11.6
	-20.71	139.49	16.29	11.54
	11.54	79.44	15.65	11.09
0	35.99	43.76	15.05	10.68



Supplementary Abstract Materials