Strength of TROPOMI observations on the retrieval of volcanic SO_2 emissions at high temporal resolution from space by inverse modeling

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Abstract

A refined knowledge of volcanic sulphur dioxide (SO_2) degassing at high temporal resolution, as SO_2 is oxidized to form sulfate aerosols in the atmosphere, is essential to advance further in understanding the consequence of volcanic emissions on air quality, ecosystems, and climate at a global scale. Concerning volcanological applications, information on SO_2 degassing remains critical for assessing the underlying magma dynamics and associated hazards. However, presently, nadir space-borne observations in the ultraviolet spectrum range, viz., OMI, GOME2, OMPS, and more recently launched TROPOMI hyperspectral sensor, can only provide snapshots of volcanic SO2 every 24 h. Here we determine hourly the SO_2 flux emissions as well as the altitude of injection by applying an inverse modeling method [1]. The forward model involves the CHIMERE Eulerian regional chemistry-transport model [2]. The idea is to evaluate the advancements in utilizing high spatially and spectrally resolved measurements from TROPOMI spectrometer onboard ESA-Sentinel-5 Precursor. This investigation focuses on the 2018 eruption of Ambrym (16.24°S, 168.15°E), a top world-ranking volcanic SO_2 emitter. It depicted a rapid cessation of a decade long SO_2 degassing and lava lake activity associated with the emplacement of a large injection of magma below the surface, crisscrossing the island of Ambrym, and spawning a submarine eruption [4].

TROPOMI assimilated CHIMERE simulation leads to more detailed information on the dispersal of the volcanic SO_2 cloud, and total mass as well as altitude of injection by the inverse modeling scheme. This provides the paroxysmal phase of the eruption occurred about 0430 UT on 15 December 2018, injecting $\sim$8 kt of SO_2 to the atmosphere at 12 km above sea level (asl). Ambrym volcano emitted $\sim$100 kt of SO_2 during 13-18 December 2018; most of the SO_2 mass was centered at 7 km altitude asl. Mostly, TROPOMI assimilated CHIMERE simulation depicts the weakest degassing of magnitude $<100\,\mathrm{t\,h^{-1}}$. At first order, SO_2 flux time series are similar using TROPOMI, GOME2, and OMPS data. Overall, TROPOMI determines better the dense parcels of SO_2 in the core of the volcanic plume than OMPS or GOME-2. As a consequence, model simulation assimilating TROPOMI observations describes better the dispersal of such dense parts of the SO2 cloud, often co-located with ash-rich zones that should be avoided for aviation safety.

Methodology

- Inverse modeling method: Linear least-squares regression approach with non-negative constraint and no a priori [1] :

$$\underbrace{\begin{pmatrix} d \\ 0 \end{pmatrix}}_{\text{Satellite Observation}} = \underbrace{\begin{pmatrix} G \\ \kappa^2\Delta \end{pmatrix}}_{\text{(Simulated) Forward Operator}} \times \underbrace{(m)}_{\text{Model Parameter}} ,$$

where κ^2 is the Lagrangian multiplier and Δ is the Laplacian - second order Tikhonov regularisation.
- Volcanic SO_2 cloud dispersal, including the physico-chemical processes, is simulated using CHIMERE (Eulerian) chemistry-transport model [2] at a large-scale during 13 to 18 December 2018.
- WRF-ARW [3] model simulation is used for forcing the meteorological fields in CHIMERE. ERA-5 reanalysis with 0.25° spatial resolution is used hourly for the initialisation and nudging at the grid boundaries of WRF-ARW simulation.
- $10\,\mathrm{km} \times 10\,\mathrm{km}$ horizontal resolution is implemented to resolve well the volcanic SO_2 dispersal, and the vertical layer thickness is maintained within 25 m to 550 m that varies as a geometric sequence.
- Gaseous tracers (passive, no aerosol chemistry) are injected each hour to the atmosphere at each kilometer in a range of 2 km to 12 km altitude asl during 2018121300 to 2018121800.
- To reproduce well the complex horizontal wind-fields, sharply varying with altitude in the surroundings of the Australian continent, WRF-ARW simulation was run with a fine vertical resolution of $\sim$250 m since 00 UT 1 December 2018 giving enough spin-up time.

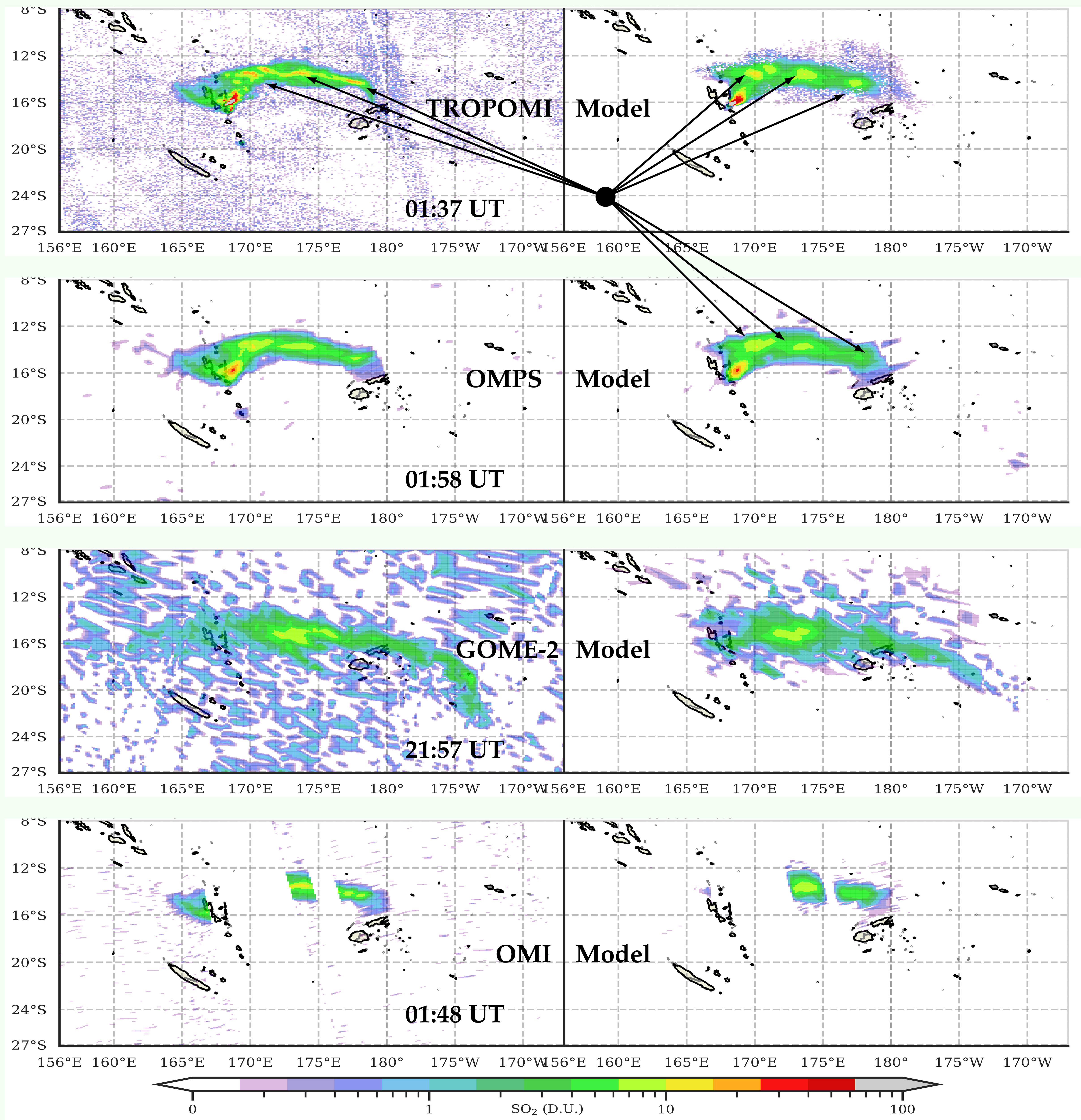
Outlook

- The high spatial and spectral resolution TROPOMI SO_2 data paves the way for the Eulerian chemistry-transport models to identify and track better the dense SO_2 parcels as well as weakest degassing by the inversion scheme. The assimilation of TROPOMI observations should improve the quality of volcanic plume forecasts that are critical for aviation safety.
- The complex wind-field, sharply changing with altitude, can impact the reconstruction of volcanic SO_2 clouds by the inverse scheme. Hence, the best available reanalysis data (e.g., ERA5) and the high-resolution meteorological model simulation are crucial to drive CHIMERE simulation.

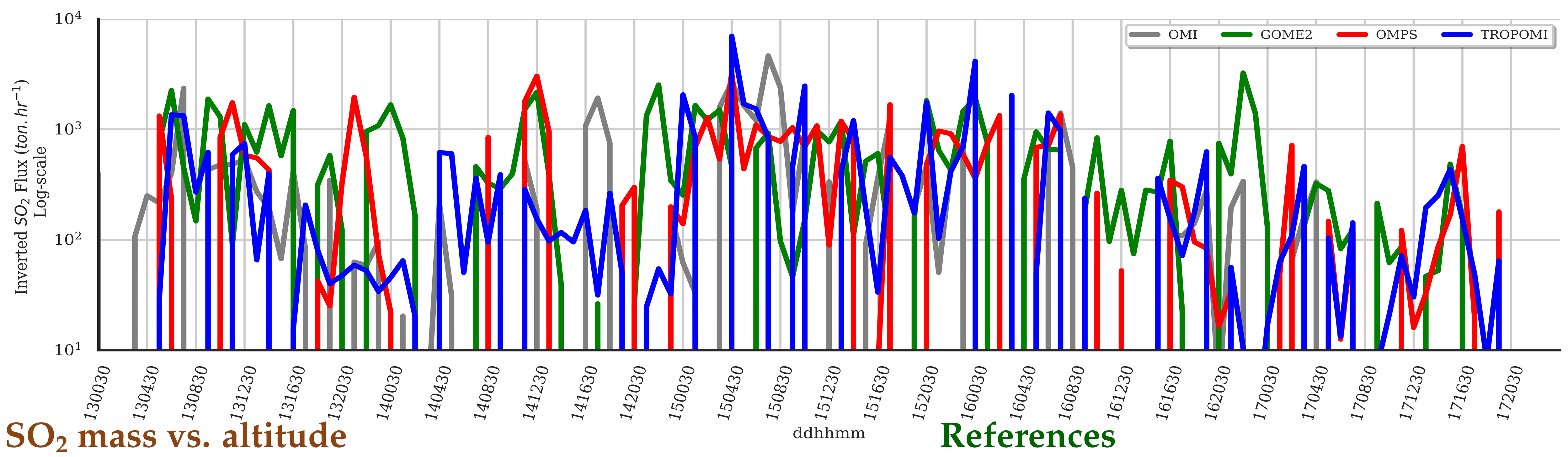
Main features of the space-borne sensors

Properties	TROPOMI	OMPS-NM	OMI	GOME2
Satellite	ESA Sentinel-5 Precursor	NOAA-Suomi NPP	NASA EOS-Aura	NOAA/ESA Metop-A+B
Spectral ranges	UV-VIS-NIR-SWIR	UV	UV-VIS	UV-VIS-NIR
Nadir spatial resolution	7 km × 3.5 km	50 km × 50 km	13 km × 24 km	80 km × 40 km
SO_2 column density retrieval	DOAS	LF	DOAS	DOAS
SO_2 detection limit (DU)	0.2	0.2	0.2	0.5
Time of overpass (local solar time)	13h30	13h30	13h30	9h30
L2 Data Source	NASA GES DISC			AC-SAF/DLR

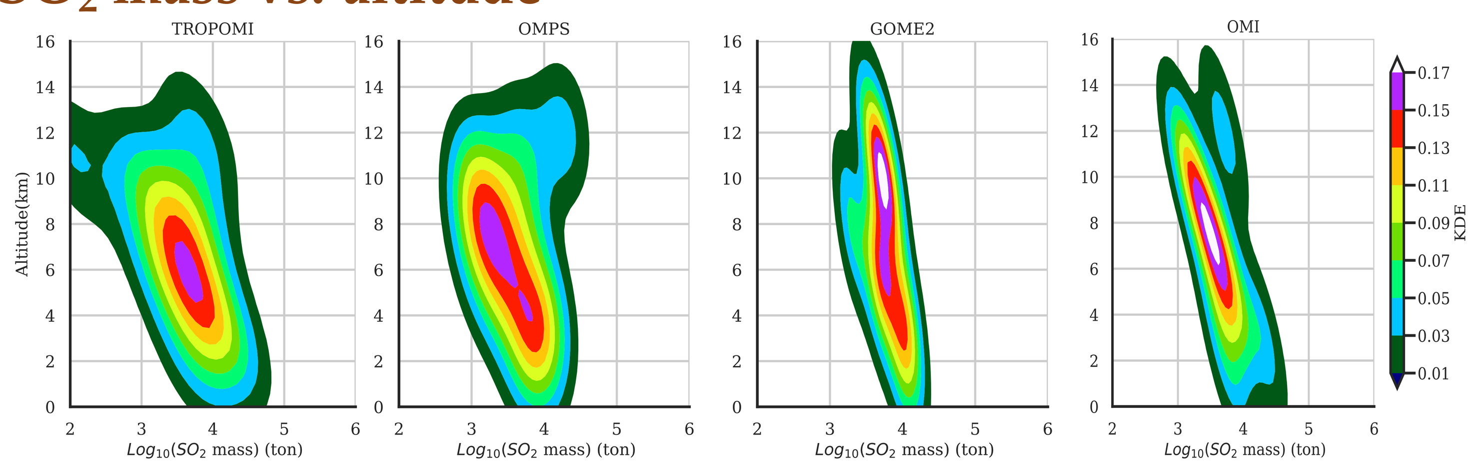
Simulation of dense volcanic SO_2 air parcels on 16 December 2018: Role of TROPOMI



Inverted SO_2 flux time series



SO_2 mass vs. altitude



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