

Investigating Differences Between IASI and TROPOMI SO₂ Retrievals Using the Scattering Reference Forward Model

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Abstract

The Infrared Atmospheric Sounding Interferometer (IASI) and the Tropospheric Monitoring Instrument (TROPOMI) can retrieve substantially different sulphur dioxide (SO₂) columns from the same volcanic plume. This study investigated the causes of this disagreement using the June 2019 Raikoke eruption. Geographically matched Level-2 retrievals were compared, while HYSPLIT trajectories were used to test the influence of observation timing and plume altitude. A nearby IASI Level-1C spectrum was then simulated using the Scattering Reference Forward Model (SRFM).

The selected measurements were 6.59 km apart, but IASI retrieved 38.17 DU compared with a height-informed TROPOMI value of 515.57 DU. Footprint averaging and trajectory analysis showed that spatial resolution and plume transport alone could not explain the difference. Optimisation produced an SRFM column of approximately 195 DU, between the two satellite retrievals. Further tests showed that the simulated IASI response depended on the conditions assumed in the model.

These results suggest that differences in retrieval sensitivity contribute to the IASI and TROPOMI disagreement. Further work should forward model TROPOMI and test additional volcanic observations.

1 Introduction

Volcanic eruptions release large amounts of gases and aerosols into the atmosphere. One of the main gases emitted is sulphur dioxide (SO₂), which can remain in the atmosphere for several days and be transported thousands of kilometres by atmospheric circulation [1]. Volcanic emissions can also affect aviation, air quality, the formation of sulphate aerosols and, following major eruptions, the Earth's climate by influencing its radiative balance [2]. Measurements of volcanic SO₂ provide information about the magnitude and evolution of an eruption.

Satellite observations allow volcanic plumes to be monitored over remote regions where ground-based observations may not be available. Two satellite instruments used to measure volcanic SO₂ are the Infrared Atmospheric Sounding Interferometer (IASI), which measures thermal infrared radiation, and the Tropospheric Monitoring Instrument (TROPOMI), which uses reflected ultraviolet radiation for its SO₂ retrieval [2, 3]. Both instruments are carried onboard polar-orbiting satellites and provide global or near-global coverage [3]. Although both instruments can observe the same volcanic plume, differences can occur between their retrieved SO₂ amounts.

These differences may arise from the different wavelength regions measured by the instruments, their sensitivity to SO₂ at different altitudes, their satellite pixel sizes, or assumptions made within the retrieval algorithms. The retrieved SO₂ amount can also be affected by the

atmospheric state and the presence of cloud or volcanic material [2].

This project investigates the causes of these differences using a high-latitude volcanic eruption observed by both IASI and TROPOMI. Level-2 SO₂ retrievals from the two instruments were compared, while the Scattering Reference Forward Model (SRFM) was used to reproduce a measured IASI Level-1 spectrum and investigate the influence of atmospheric and volcanic parameters. The overall aim is to identify the physical factors that may explain the disagreement between IASI and TROPOMI SO₂ retrievals.

2 Method

2.1 Satellite instruments and SO₂ retrievals

IASI and TROPOMI can both detect volcanic SO₂, but they measure different types of radiation and use different methods to estimate the amount of SO₂. Neither instrument directly measures a final SO₂ column; instead, satellite measurements are processed using retrieval algorithms to estimate the amount of SO₂ in the atmosphere.

IASI is an infrared instrument onboard the Metop satellite series. It orbits at approximately 800 km and provides near-global coverage twice per day. It measures thermal infrared radiation emitted by the Earth and atmosphere between 645 and 2760 cm⁻¹ [4]. Volcanic SO₂ produces spectral features around 1150 and 1360 cm⁻¹, which can be used to estimate the amount of SO₂ present [5]. The Level-1C product contains the measured spectra, while the Level-2 product contains retrieved values, including SO₂ column and plume altitude. Atmospheric and surface temperatures are important because thermal contrast affects the performance of the IASI SO₂ retrieval [6].

TROPOMI is an imaging instrument onboard Sentinel-5 Precursor, orbiting at approximately 824 km and providing global coverage once per day. Its SO₂ retrieval mainly uses reflected ultraviolet sunlight in the 312–326 nm

range [7]. It first estimates the amount of SO₂ along the path travelled by the light, known as the slant column. This is converted into a vertical SO₂ column using an air mass factor, which accounts for viewing angle, clouds, surface properties and the assumed height of the SO₂ [7]. TROPOMI can also estimate SO₂ layer height for strong volcanic plumes [8].

The main difference is therefore that IASI uses thermal infrared radiation, while TROPOMI uses reflected ultraviolet sunlight. Their different wavelengths and retrieval methods give them different sensitivities to plume height and atmospheric conditions, which may contribute to differences between their retrieved SO₂ amounts.

2.2 Satellite data and case study

The June 2019 eruption of Raikoke volcano in the Kuril Islands was selected because it produced a large, high-altitude SO₂ plume observed by both instruments. The eruption began at approximately 18:05 UTC on 21 June and released gases into the upper troposphere and stratosphere [8, 9].

IASI Metop-A Level-2 SO₂ data were obtained from the Université libre de Bruxelles/Laboratoire Atmosphères, Milieux, Observations Spatiales (ULB/LATMOS) volcanic SO₂ product distributed through the AERIS atmospheric Data and Service Centre [11]. This provided SO₂ column, plume altitude, location and observation information. IASI Level-1C spectra were also used for forward modelling. TROPOMI Sentinel-5P Level-2 SO₂ data were obtained from the Copernicus Sentinel data service and provided SO₂ vertical column, coordinates, observation time and quality-assurance (`qa_value`) information [10].

Measurements from 22 June were selected. The analysed IASI observation occurred at 00:06:55 UTC and TROPOMI at 02:21:51 UTC, approximately 2 h 15 min later. Their SO₂ columns were mapped at the satellite coordinates to compare the plume distributions and select representative measurements for further analysis.

2.3 Geographical plume analysis

The Level-2 products were processed in Python and geographically restricted to the Raikoke plume region. The representative TROPOMI SO₂ pixel was selected using `qa_value` ≥ 0.5 , following the recommended threshold for excluding lower-quality retrievals affected by factors such as cloud. TROPOMI columns were converted from mol m⁻² to Dobson Units (DU), using $1 \text{ mol m}^{-2} \approx 2241 \text{ DU}$ [10].

Both datasets were plotted at their original satellite coordinates. The highest-SO₂ TROPOMI pixel remaining after quality filtering was selected because it represented the strongest part of the plume. It was geographically matched to the closest IASI Level-2 measurement, without requiring the IASI measurement to have a similarly high SO₂ value. Because the observations were not exactly simultaneous, atmospheric transport was subsequently investigated using HYSPLIT.

To determine whether the selected comparison was representative of the wider plume, each positive IASI Level-2 retrieval was first matched to its nearest TROPOMI pixel. TROPOMI pixels ($3.5 \times 7 \text{ km}$) within 6.5 km of each approximately 12 km IASI footprint centre were averaged [4]. Correlation, bias and root-mean-square error were calculated for the matched retrievals. This analysis was performed for 22, 23 and 24 June and 1 July to test whether the relationship between the instruments remained consistent as the plume evolved. Bias was defined as the mean IASI column minus the mean TROPOMI column.

The IASI Level-1C spectrum used for the SRFM analysis came from a different IASI measurement. It was selected because it was the closest available Level-1C spectrum to the strong TROPOMI plume location, approximately 6.6 km away, and therefore sampled a nearby part of the same plume.

2.4 Plume altitude analysis

The vertical position of the plume was investigated using the SO₂ altitude retrieval included

in the IASI ULB/LATMOS Level-2 AERIS product [11]. The retrieved altitude of the IASI pixel selected for forward modelling was recorded, and surrounding SO₂-containing pixels were also analysed to determine whether this altitude was representative of the wider plume. The distribution, range and median of the retrieved altitudes were calculated. These independent Level-2 altitude estimates were later compared with the plume altitudes tested using SRFM, allowing the altitude that best reproduced the measured IASI spectrum to be assessed against the satellite retrieval.

2.5 HYSPLIT trajectory analysis

The Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model was used to investigate plume movement. HYSPLIT uses meteorological wind fields to calculate the expected path of an air parcel through the atmosphere.

A forward trajectory from the earlier IASI observation and a backward trajectory from the later TROPOMI observation were first used to test whether their locations could be explained by plume movement. A second analysis used Raikoke at the eruption start time (18:05 UTC, 21 June 2019) as a common starting point. Forward trajectories using GDAS 1° meteorological data were calculated at 9, 17 and 22 km to test how plume height affected its movement. Predicted positions at the IASI and TROPOMI observation times were then compared with the observed locations.

2.6 IASI forward modelling using SRFM

The Scattering Reference Forward Model (SRFM) is a one-dimensional line-by-line radiative-transfer model developed by the Oxford Earth Observation Data Group [12]. It combines the Reference Forward Model (RFM), which calculates gaseous absorption and emission, with DISORT, which calculates radiative transfer including particle scattering. SRFM can therefore simulate the top-of-

atmosphere spectrum that would be observed by an infrared instrument such as IASI.

An IASI Level-1C spectrum close to the selected plume location was used as the measured reference. Its radiances were converted to brightness temperature and compared directly with SRFM brightness-temperature simulations. The simulations were used to test how changes in the volcanic plume and surrounding atmosphere affected the IASI spectrum. These tests included changing the amount and altitude of SO₂, as well as the atmospheric temperature structure such as water vapour and ozone. Moreover, cloud properties and volcanic particles were also investigated because they can alter the infrared radiation reaching the satellite.

Agreement was quantified using the root-mean-square error,

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (T_{\text{IASI},i} - T_{\text{SRFM},i})^2}, \quad (1)$$

where N is the number of spectral points. RMSE was calculated across the wider spectrum and separately within SO₂-sensitive regions, with lower values indicating closer agreement.

Finally, using an evolution differential optimiser algorithm, SO₂ parameters such as the plume thickness were optimised simultaneously to determine the best-fitting combination. The initial standard atmospheric temperature profile was also replaced with conditions representative of the IASI observation to test the sensitivity of the solution to the assumed atmospheric state. The resulting solutions were compared with the independent IASI Level-2 retrieval.

3 Results

3.1 IASI and TROPOMI SO₂ comparison

The geographical distributions of the Raikoke SO₂ plume observed by IASI and TROPOMI

are shown in (Fig. 1). The selected measurements were geographically close, with the IASI and TROPOMI pixels approximately 6.59 km apart, but their retrieved SO₂ amounts differed strongly (Table 1). IASI retrieved 38.17 DU, compared with the default TROPOMI vertical column of 3543.99 DU, which was calculated using the product’s standard assumption about the vertical distribution of SO₂. The selected TROPOMI measurement was the highest-SO₂ pixel remaining after quality filtering.

TROPOMI also retrieved an SO₂ layer height of approximately 9.4 km. This observation-specific height was used to select the corresponding height-dependent TROPOMI column instead of relying on the standard vertical-profile assumption. The resulting column decreased to 515.57 DU. Although this reduced the disagreement considerably, the TROPOMI value remained approximately 13.5 times larger than the IASI retrieval.

Table 1: Selected plume measurements on 22 June 2019.

	IASI	TROPOMI	TROPOMI _{LH}
Lat. (°N)	48.4448	48.3896	48.3896
Lon. (°E)	155.5106	155.4781	155.4781
Time (UTC)	00:06:55	02:21:51	02:21:51
SO ₂ (DU)	38.17	3543.99	515.57
Height (km)	17.0	–	9.40

3.2 Wider plume comparison

The comparison was extended across the plume using footprint-matched measurements, with the results summarised in (Table 2) and (Fig. 2). On 22 June, 115 matches were obtained, with a mean SO₂ column of 10.48 DU for IASI and 337.58 DU for TROPOMI. The correlation was 0.397, while the bias of –327.1 DU and RMSE of 855.7 DU showed that the retrieved amounts remained substantially different.

The mean columns were much closer on the later dates, but the spatial agreement remained weak. On 24 June, for example, the mean columns were 2.70 DU for IASI and 2.59 DU

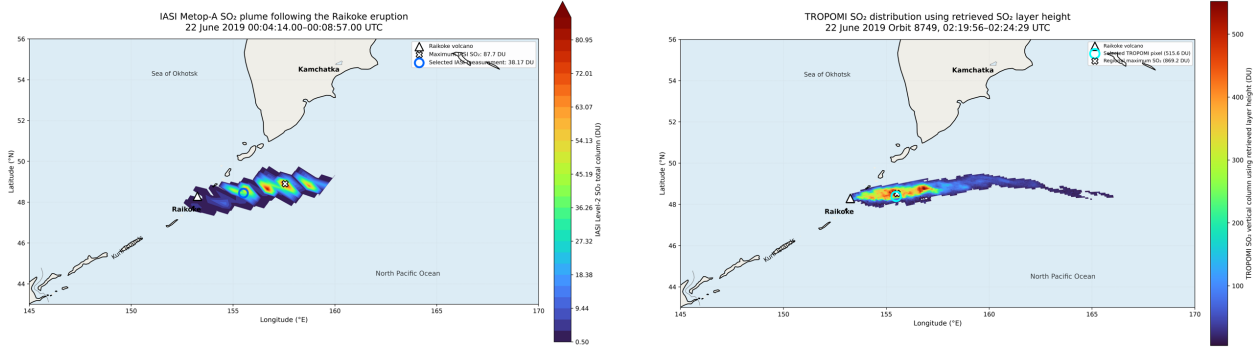


Figure 1: Geographical distribution of the Raikoke SO₂ plume observed by IASI (left) and TROPOMI (right) on 22 June 2019. Colour indicates the retrieved SO₂ column in Dobson Units (DU), while the circles indicate the measurements selected for comparison.

for TROPOMI, despite a correlation of -0.132 . Similar mean values therefore did not necessarily mean that the instruments retrieved the same spatial distribution. Overall, the relationship varied between observations rather than following a constant bias.

3.3 Plume altitude and atmospheric transport

The geographical comparison showed an unexpected result: although TROPOMI observed the plume later than IASI, its selected measurement was not farther downwind. This meant that the difference between the satellite observations could not be explained simply by assuming that the same plume had moved between the two overpasses.

Plume height was therefore considered because winds vary with altitude. IASI retrieved a height of 17 km for the selected measurement, representing its estimate of the altitude of the SO₂ layer rather than the altitude at which the greatest SO₂ amount occurred. The retrieved heights of 28 nearby IASI plume measurements ranged from 3–17 km, with a median of 11 km. HYSPLIT trajectories were started at 9, 17 and 22 km, representing the approximate TROPOMI height, the IASI-retrieved height and a higher plume scenario. They predicted very different transport paths (Fig. 3). Although the 9 km trajectory was more closely aligned with the general direction of the ob-

served plume, the 17 km trajectory gave the closest predicted positions at the satellite observation times. Its predicted position was approximately 89 km from the IASI measurement and 83 km from the TROPOMI measurement. Therefore, none of the trajectories reproduced the observed plume locations precisely.

The time difference and altitude-dependent transport therefore affect the comparison, but do not by themselves explain why TROPOMI retrieved 515.57 DU while IASI retrieved only 38.17 DU. The IASI spectrum was therefore modelled with SRFM to test whether plume altitude and other atmospheric assumptions could explain the remaining SO₂ difference.

3.4 SRFM sensitivity to SO₂ concentration and altitude

The measured IASI Level-1C spectrum was converted from radiance to brightness temperature and compared with SRFM simulations. SO₂ concentration and plume altitude were initially varied independently, while agreement with IASI was assessed using RMSE in the SO₂-sensitive spectral regions. The effect of changing plume altitude is shown in (Fig. 4).

Increasing the SO₂ concentration changed the strength of the spectral features, while changing plume altitude altered the simulated IASI response through its effect on thermal contrast. However, neither parameter alone reproduced the measured spectrum across the

Table 2: Statistical comparison of spatially matched IASI and TROPOMI SO₂ retrievals. Bias is defined as IASI minus TROPOMI.

Date	Matches	Mean IASI (DU)	Mean TROPOMI (DU)	Correlation	Bias (DU)	RMSE (DU)
22 Jun	115	10.48	337.58	0.397	-327.1	855.7
23 Jun	10	1.98	0.57	0.172	+1.41	2.19
24 Jun	99	2.70	2.59	-0.132	+0.12	3.65
1 Jul	26	0.20	0.59	0.040	-0.39	0.50

full spectral region. This indicated that the IASI retrieval could not be explained by SO₂ amount alone and that the surrounding atmospheric conditions also needed to be considered.

3.5 Optimised SRFM simulation

The initial simulations showed that several atmospheric parameters affected the spectral fit. A differential-evolution optimiser was therefore used first to fit the background atmosphere by varying temperature, water vapour, ozone and volcanic-cloud properties. An initial solution placed liquid-water cloud at approximately 17 km, which was physically unrealistic, so it was replaced with an ice-cloud representation and the atmosphere was re-optimised.

After fixing the optimised background, SO₂ concentration, altitude and layer thickness were fitted within the ν_1 and ν_3 SO₂ bands. The final solution contained 6.76 ppmv of SO₂, centred at 22.5 km with a thickness of 5.07 km. This corresponded to approximately 195 DU, between the IASI Level-2 value of 38.17 DU and the height-informed TROPOMI value of 515.57 DU. The result shows that the model representation can substantially alter the SO₂ column inferred from the IASI spectrum, helping to narrow, but not close, the IASI-TROPOMI difference. The resulting spectral fits are shown in (Fig. 5).

3.6 Observation-specific atmospheric and cloud sensitivity

The robustness of the optimised solution was tested using conditions specific to the IASI ob-

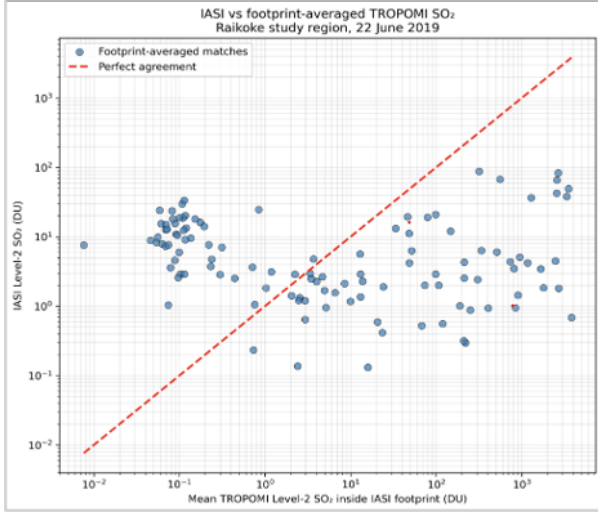
servation, as shown in (Fig. 6). The optimised atmosphere was replaced with a local atmospheric profile, while the reported 100% cloud cover was represented using an ice cloud at approximately 232 K. SO₂ was held fixed at approximately 6 ppmv to isolate the influence of the atmospheric and cloud assumptions.

Changing these conditions altered the simulated IASI spectrum despite the fixed SO₂ concentration. This demonstrates that the IASI spectral response depends on how the plume, atmosphere and cloud are represented. These sensitivities may therefore contribute to the different SO₂ amounts retrieved by IASI and TROPOMI, although the TROPOMI spectrum would need to be forward modelled to test this directly.

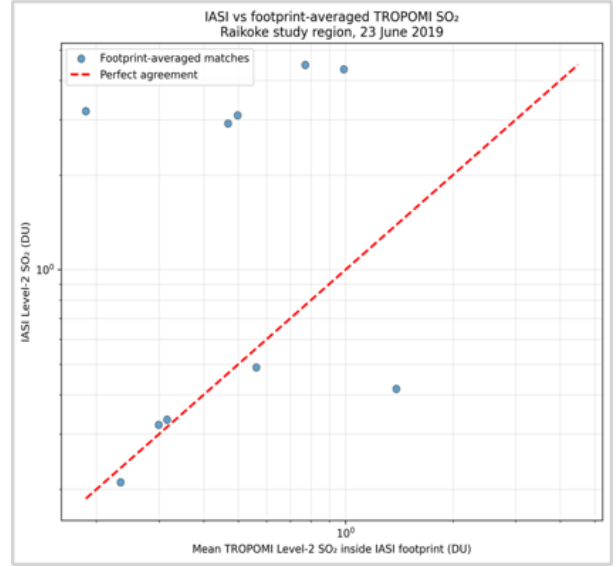
4 Discussion

The results show that no single factor fully explains the IASI and TROPOMI disagreement. Raikoke was a useful case study because its strong, high-altitude plume was observed by both instruments within approximately 2 h 15 min, allowing their retrievals to be compared over the same volcanic event.

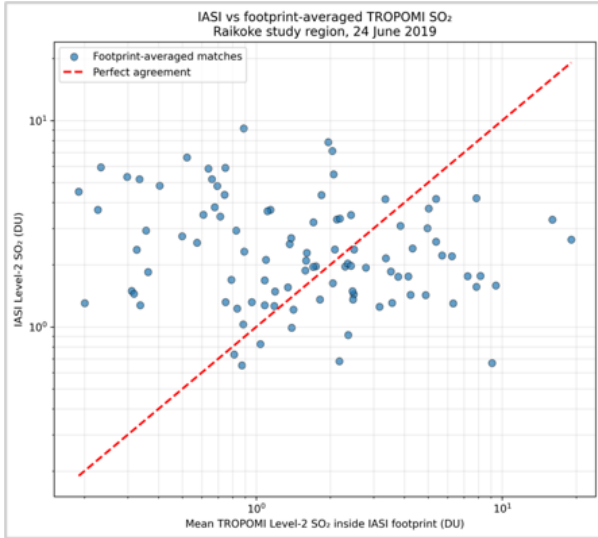
The geographical analysis showed that the disagreement was not limited to the selected pixel pair. Footprint averaging reduced the effect of the different spatial resolutions, but large differences remained, and the relationship between the retrievals varied between dates. This suggests that the Raikoke discrepancy was not a simple fixed bias. However, a single eruption cannot establish whether similarly large differences occur systematically for all IASI



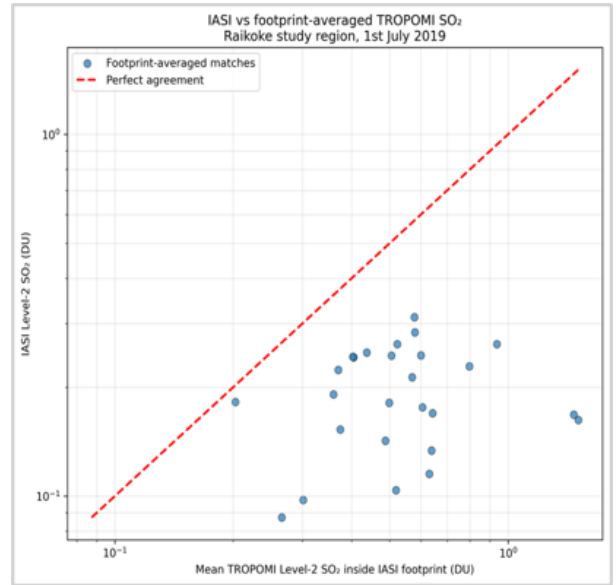
(a) 22 June 2019



(b) 23 June 2019



(c) 24 June 2019



(d) 1 July 2019

Figure 2: Spatial comparison of footprint-matched IASI and TROPOMI SO_2 retrievals following the Raikoke eruption.

and TROPOMI observations.

The HYSPLIT results showed that the predicted direction of plume movement changed with altitude, but could not account for the large difference between the retrieved SO_2 columns. The 9 km trajectory was more closely aligned with the general direction of the observations, whereas the 17 km trajectory pro-

duced the closest positions at the satellite observation times. However, none of the trajectories reproduced the observed locations precisely. The observation-time difference may therefore have contributed to the spatial mismatch, but it is unlikely to be the main cause of the retrieval disagreement.

The SRFM analysis provided the clearest in-

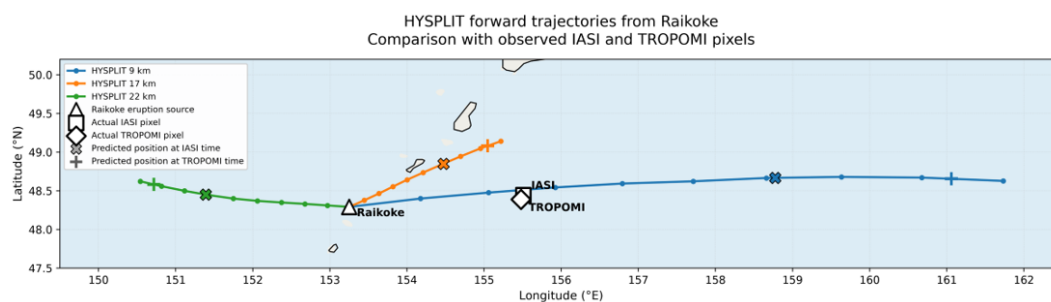


Figure 3: HYSPLIT forward trajectories from Raikoke at 9, 17 and 22 km, with predicted plume positions at the IASI and TROPOMI observation times compared with the observed satellite locations.

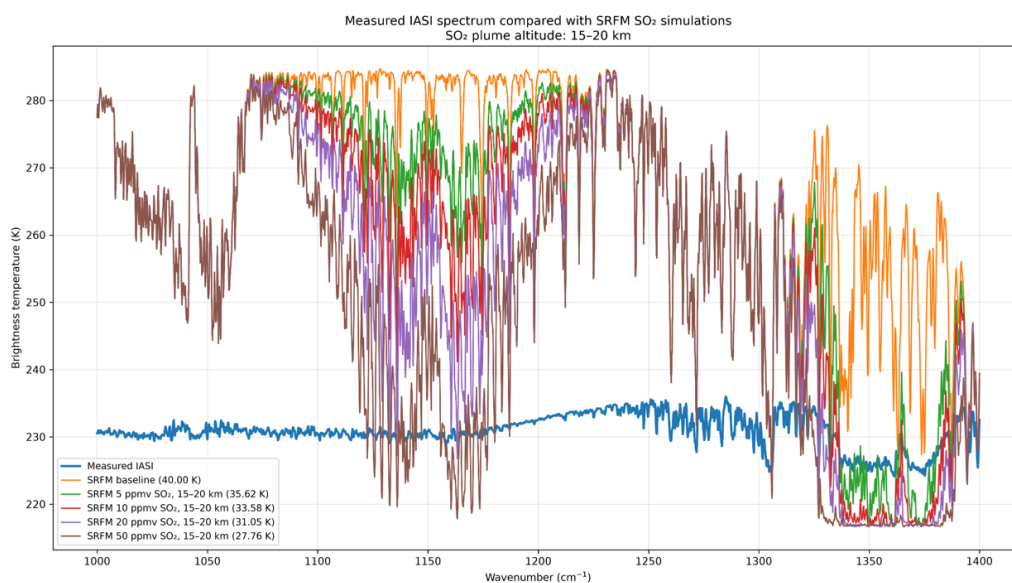


Figure 4: Measured IASI brightness-temperature spectrum compared with SRFM simulations using different SO₂ plume altitudes.

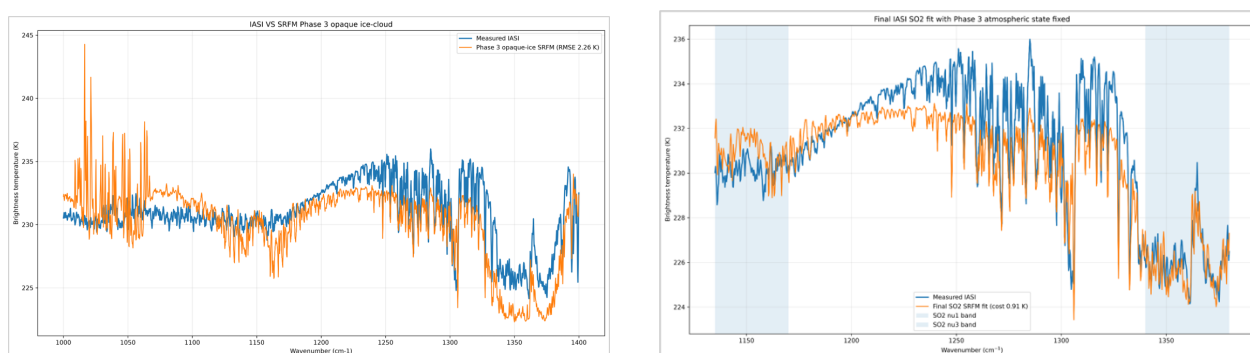


Figure 5: Measured IASI spectrum compared with the SRFM simulation following optimisation of the background atmosphere (left) and the SO₂ parameters within the ν_1 and ν_3 bands (right).

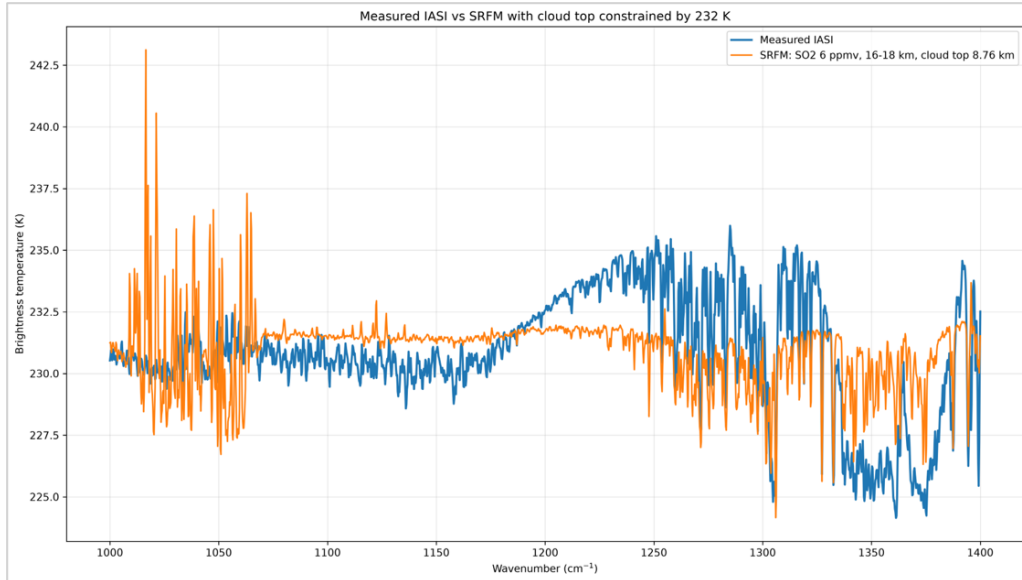


Figure 6: Measured IASI spectrum compared with the SRFM simulation using a local atmospheric profile and observation-specific cloud conditions, with SO_2 fixed at approximately 6 ppmv.

sight into the IASI retrieval. The optimised simulation produced approximately 195 DU, between the IASI Level-2 value of 38.17 DU and the height-informed TROPOMI value of 515.57 DU. The sensitivity tests showed that the IASI spectrum depended on the assumed plume altitude and atmospheric and cloud conditions. The disagreement may therefore be partly related to how the instruments' infrared and ultraviolet retrievals respond to the structure and conditions of the same plume.

5 Limitations

The detailed spectral analysis was based on one primary plume case, so it cannot determine whether the discrepancy is systematic across other volcanic eruptions or under different atmospheric conditions.

Different combinations of plume and atmospheric parameters may produce similarly good fits to the measured spectrum. Therefore, the optimised values should not be treated as a unique solution. The SRFM also modelled the atmosphere above one location and did not represent variations across the satellite footprint.

Furthermore, only the IASI spectrum was

forward modelled. TROPOMI was analysed using its retrieved Level-2 values, so this study could not directly determine how TROPOMI's retrieval assumptions affected its SO_2 result.

6 Conclusion

The large difference between the IASI and TROPOMI SO_2 retrievals remained after accounting for the instruments different spatial resolutions. The time between the observations and the expected movement of the plume also did not fully explain it. SRFM retrieved an SO_2 column between the two satellite values and showed that the IASI response depended strongly on the representation of the plume and atmosphere. The instruments different retrieval sensitivities are therefore likely to be an important source of the disagreement.

Future work should forward model the TROPOMI ultraviolet measurement so that both instruments can be tested directly. Applying the analysis to more observations would show whether the Raikoke discrepancy is part of a wider pattern or specific to this plume.

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