First BrO retrievals and small-scale enhancement analysis in the Arctic using TROPOMI/S5P

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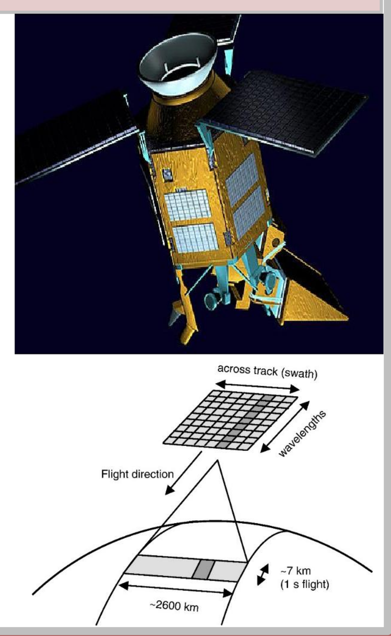
1. Introduction

Satellite observations from instruments such as GOME, SCIAMACHY, GOME-2 and OMI have been used for monitoring of bromine monoxide (BrO) distributions on regional to global scales for more than two decades. To continue and improve daily global trace gas observations with an unprecedented spatial resolution, the TROPOspheric Monitoring Instrument (TROPOMI) was launched onboard the Copernicus Sentinel-5 Precursor platform in October 2017 (Veefkind et al., 2012). In this study, sensitivity tests were performed to find an optimal retrieval wavelength range for TROPOMI DOAS BrO retrievals under various measurement conditions. From these sensitivity tests, a wavelength range for TROPOMI BrO retrievals was determined and several case studies were retrieved. The examples of individual TROPOMI overpasses show that due to the better signal to noise ratio and finer spatial resolution of 3.5x7 km^2, TROPOMI BrO retrievals provide good data quality with low fitting errors and unique information on small scale variabilities in various BrO source regions.

2. Sentinel-5 Precursor (S-5P)/TROPOMI

The ESA (European Space Agency) Sentinel-5 Precursor (S-5 P) is a low Earth orbit polar satellite that was launched in October 2017 to provide daily global information on columns of trace gases and aerosols.
The TROPOspheric Monitoring Instrument (TROPOMI) is a spectrometer on board of the S-5P satellite platform with spectral bands in the UV, VIS, NIR and SWIR. This wavelength range can measure key atmospheric constituents including O_3, NO_2, SO_2, CO, CH_4, HCHO, BrO and aerosol properties. The instrument has a large swath of 2600 km with high spatial resolution of currently 3.5x7 km^2 at nadir. Compared to previous satellites, TROPOMI has prominent advantages in extended spectral band range and higher spatial resolution.



3. BrO retrieval from TROPOMI

▪ DOAS retrieval

The retrieval algorithm for BrO uses the Differential Optical Absorption Spectroscopy (DOAS) technique. The absorber concentration integrated along the light path, the slant column density (SCD), is determined assuming the Beer-Lambert's law is applicable.

$$I(\lambda, s) = I_0 exp(-\sigma(\lambda)\rho s)$$

(the initial intensity: I_0, the length of light path: s, the absorption cross-section: σ, the absorber number density: ρ)
BrO SCD retrievals are typically performed within the wavelength range from 320 to 364 nm which covers 9 absorption peaks of BrO

▪ Sensitivity test of retrieval fitting intervals

- Selection of the retrieval fitting window is one of the most important things in the DOAS retrieval process
- Sensitivity tests of the wavelength interval on DOAS BrO retrievals were performed by evaluating the BrO SCDs and fitting RMS values in many different wavelength
- Start (End) limits of retrieval wavelength : 320–338 nm (342–364 nm)
- Wavelength interval step : 0.2 nm - Polynomial of order 4
- BrO, O_3, NO_2, HCHO, OClO, O_4 and Ring cross sections

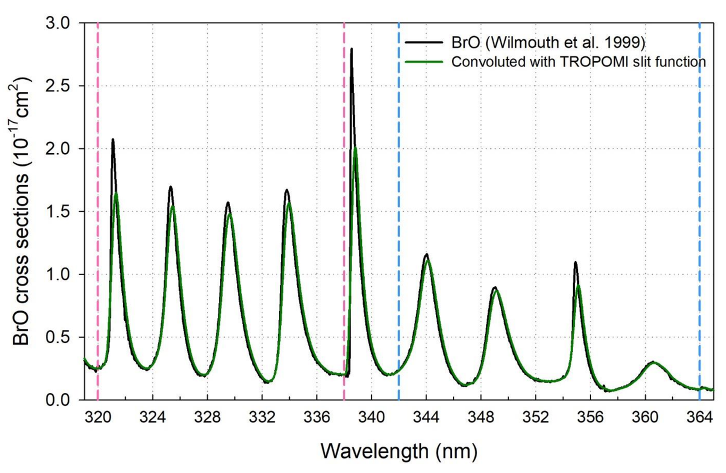


Figure 1. BrO absorption cross-section at 228 K (Wilmouth et al., 1999) used in the DOAS BrO retrieval study. The green line is the BrO cross-section convoluted by the TROPOMI slit function. Pink vertical dashed lines indicate start wavelength ranges and blue lines end wavelength ranges of fitting windows

Table 1. Geographical and time information for the different scenarios of the sensitivity tests

	Latitude [°]	Longitude [°]	Date	No. of pixel
Polar sea ice	72.5±2.5	200.0±20.0	Mar 17 2018 (orbit# 2206)	31261
Salt marsh	24.0±0.3	70.0±0.5	Mar 31 2018 (orbit# 2397)	113
Volcanic plume	-16.0±1.0	169.0±1.0	Nov 17 2017 (orbit# 492)	1748
Clear ocean	-7.0±1.0	-140.0±14.0	Apr 9 2018 (orbit# 2533)	14254
Cloudy scene	-3.0±1.0	-142.0±14.0	Apr 9 2018 (orbit# 2533)	14255

▪ BrO retrievals over the polar sea ice region

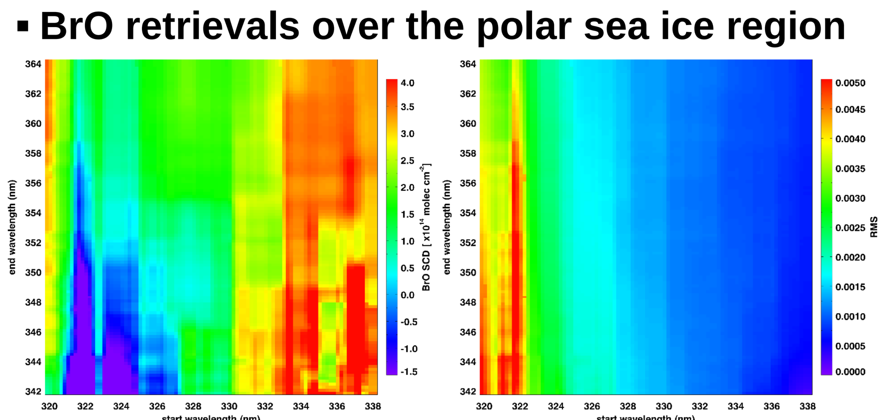


Figure 2. Colour coded means of BrO SCDs (left) and fitting RMS values (right) retrieved over the selected Arctic sea ice region for a BrO explosion event using TROPOMI measurements at different wavelength intervals

- Negative BrO SCDs with relatively high fitting RMS values at shorter wavelength < 327 nm
- The retrieval wavelength intervals with a start limit > 333.4 nm : low O_3 interference, realistic values with low fitting RMS

▪ BrO retrievals over a salt marsh

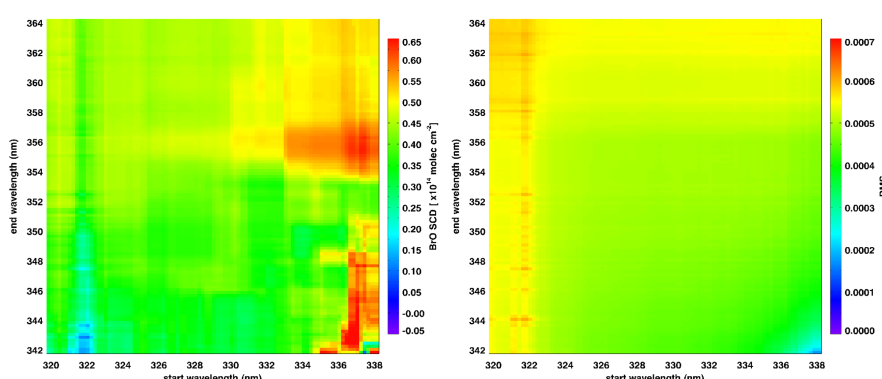


Figure 3. As Fig. 2 but for the Rann of Kutch salt marsh

- Relatively high fitting RMS values at wavelength <322 nm
- High BrO SCDs with low fitting errors : wavelength range at start limits of 333-338 nm and end limits of 354-364 nm

▪ BrO retrievals over clear scenes in the Pacific background region

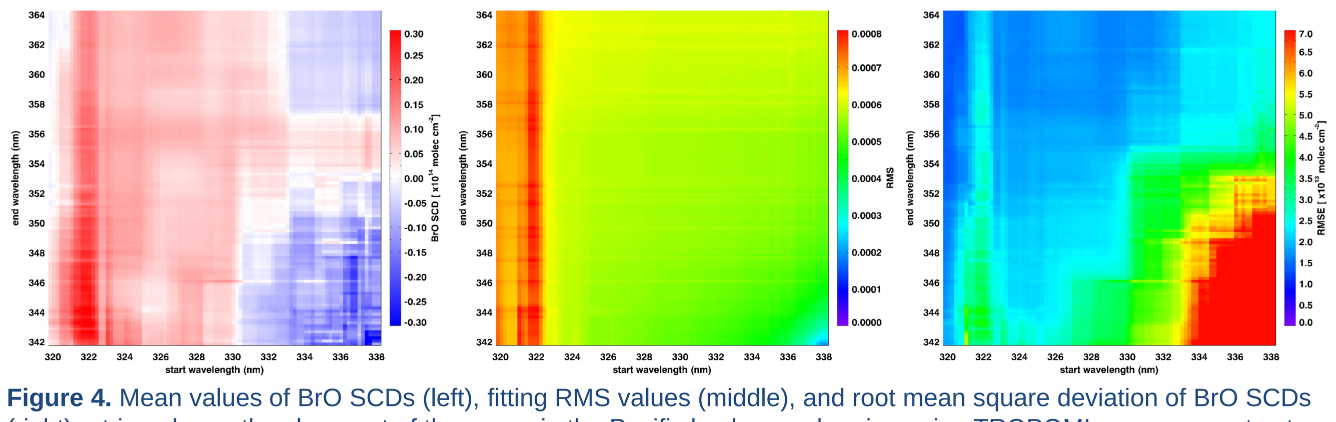


Figure 4. Mean values of BrO SCDs (left), fitting RMS values (middle), and root mean square deviation of BrO SCDs (right) retrieved over the clear part of the scene in the Pacific background region using TROPOMI measurements at different wavelength intervals.

- As this area is located within the background region used for the mean background spectrum, the retrieved BrO SCDs are close to the detection limit
- The RMSE value represents the scatter of the BrO SCDs around the true BrO SCD -> lower RMSE value indicates a better retrieval result with reduced uncertainty on the slant column
- High fit errors occur at wavelength < 322.6 nm due to the influence of absorption by stratospheric O_3

▪ BrO retrievals over cloudy scenes in the Pacific background region

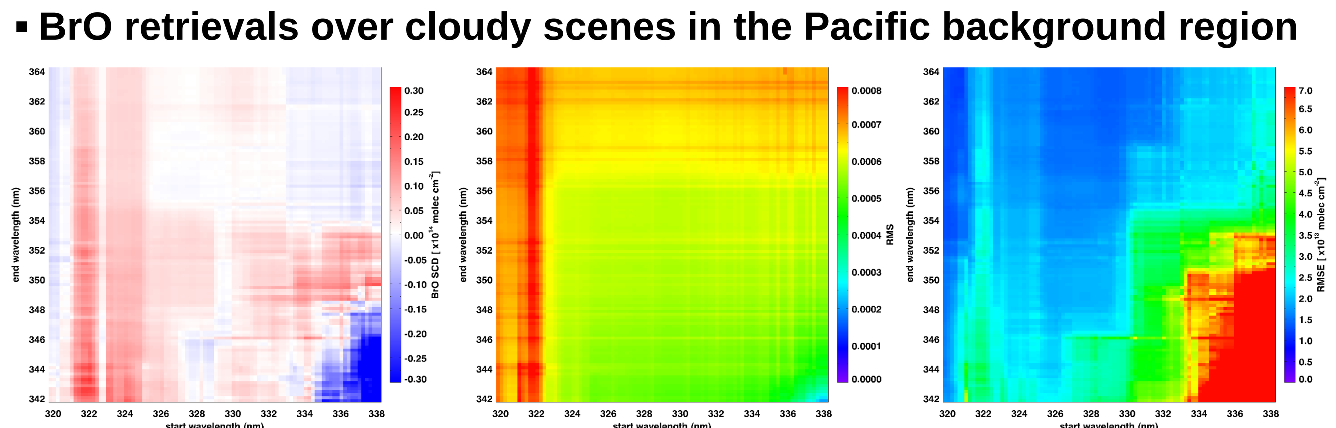


Figure 5. As Fig. 4 but for the cloudy part of the Pacific background region

- The retrieved BrO SCDs in the cloudy scene are closer to the true value (0) than in the clear scene measurement scenario
- The RMSEs for the cloudy sky measurement scenario is lower than for the clear sky case
- Cloudy sky measurement scenarios show relatively higher fitting RMS values at wavelengths longer than 358 nm due to the Ring effect

▪ DOAS settings used for the BrO retrievals

Parameter	Description
Fitting window	333.5 – 357 nm
Solar Reference Spectrum	Kurucz solar spectrum (Fraunhofer calibration)
Trace gases cross sections	BrO (Wilmouth et al., 1999; 228K) O_3 (Serdyuchenko et al., 2013; 223K, 243K) NO_2 (Vandaele et al., 1998; 220K) OClO (Kromminga et al., 2003; 213K) O_4 (Hermans et al., 298K) HCHO (MellerMoortgat et al., 2000 ;298K)
Ring cross sections	Ring cross section calculated by SCIATRAN model
Polynomial	5 coeff
Background	For TROPOMI and OMI one spectrum per row, daily averaged earthshine spectrum in selected Pacific region
Offset correction	Linear offset (2 parameters)

- The optimal retrieval fitting windows can be defined as those wavelength intervals which show higher BrO signals with lower fitting residuals in the BrO source regions, while the BrO SCDs should be minimal with narrow distributions of SCDs over the clean Pacific background region
- Fitting windows with a start limit above 327 nm are preferred to avoid strong O_3 and SO_2 interferences
- Fitting windows with an end limit less than 362 nm are recommended due to less impact of Ring effect resulting from clouds and/or high aerosol loads

▪ Comparison to OMI and GOME-2B retrievals

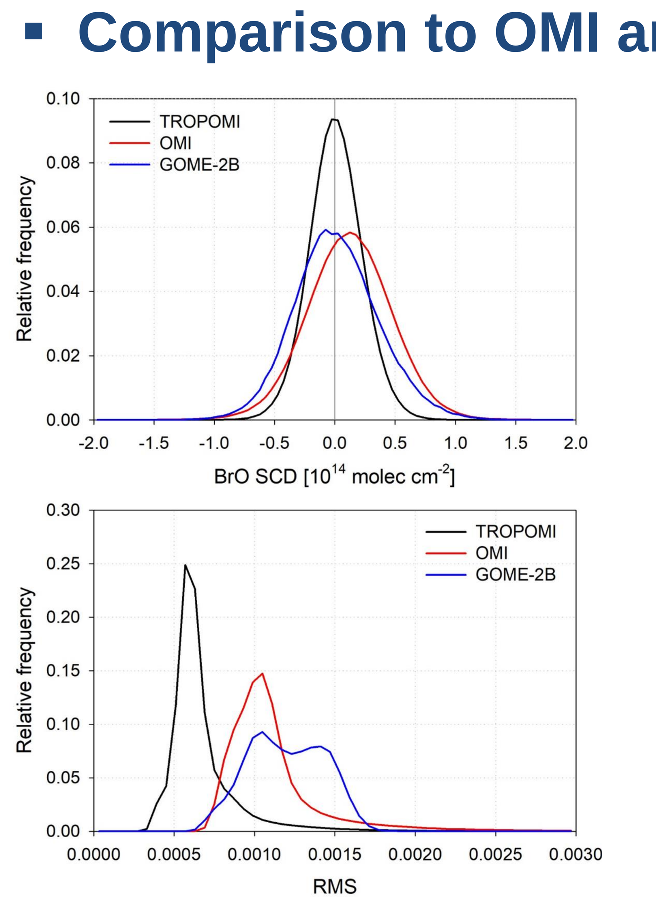


Fig 6. Distribution of BrO SCDs and fitting RMS values over a clean equatorial Pacific region (10°S-10°N, 150-260°E) for April 2018

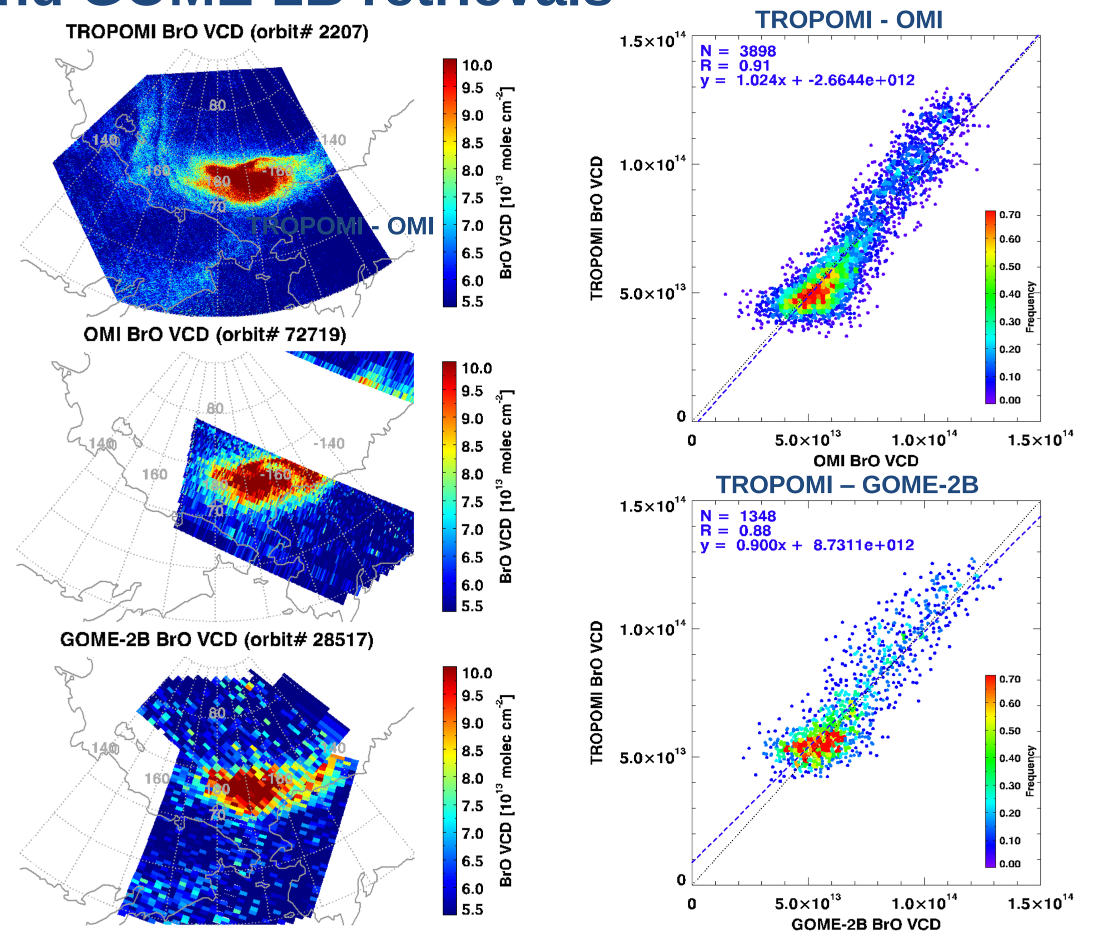


Fig 7. Scatter plots of TROPOMI and OMI BrO vertical columns, TROPOMI and GOME-2B BrO vertical columns in the selected region of enhanced BrO plumes on March 17, 2018

▪ BrO plumes over Arctic sea ice

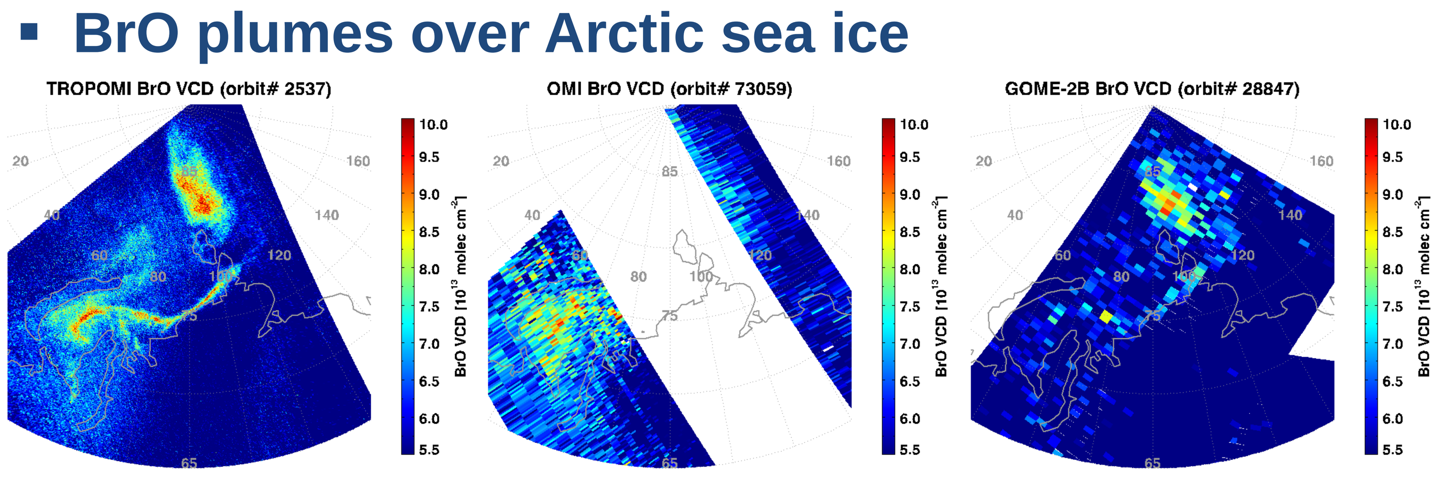


Fig 8. BrO geometric vertical columns observed over the Arctic sea ice region on 10 April 2018 by TROPOMI (left), OMI (middle) and GOME-2B (right)

- A small compact BrO enhancement as well as a long BrO plume extending along the coastline
- The long and thin enhanced BrO plume near the coastline is prominent in the map of TROPOMI

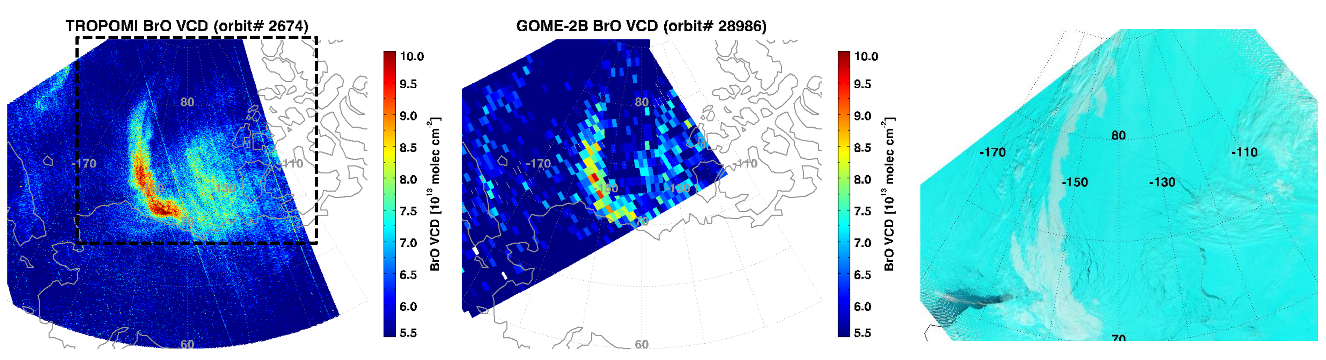


Fig 9. BrO geometric vertical columns observed over the Arctic sea ice region on 19 April 2018 by TROPOMI (left), GOME-2B (middle) and MODIS image using combinations of 7-2-1 bands (right)

- The enhanced BrO plume appears to be similar to the development of open leads in the sea ice as shown in the MODIS image
- Small-scale BrO explosion events around open leads or polynyas can be better investigated using TROPOMI

4. Conclusions / Outlook

- In this study, we present retrievals of BrO column amounts from TROPOMI observations using an optimized and adapted DOAS retrieval algorithm.
- TROPOMI shows excellent performances with much smaller fitting RMS values and lower random scatter of BrO columns than OMI and GOME-2B.
- TROPOMI BrO retrievals show good agreements with OMI and GOME-2B BrO columns.
- More small-scale hotspots can be identified in greater detail by TROPOMI with its improved signal-to-noise ratio and the excellent spatial resolution of 3.5x7 km^2.
- Stratospheric correction schemes and more sophisticated air mass factor calculations accounting for factors such as presence of clouds, varying surface albedo, and surface altitude are needed to obtain accurate tropospheric BrO columns.
- In addition to the satellite inter-comparisons, validation with ground-based measurements should be performed for more detailed assessment of the quality of TROPOMI BrO columns.

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▪ References

- VEEFKIND, J. P., et al. TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. Remote Sensing of Environment, 2012, 120: 70-83.
- VOGEL, L., et al. Retrieval interval mapping: a tool to visualize the impact of the spectral retrieval range on differential optical absorption spectroscopy evaluations. Atmospheric Measurement Techniques, 2013, 6.2: 275-299