BrO Algorithm document

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Forward model

The radiative transfer model (RTM) used and viewing geometry conventions are described in McLinden *et al.* [2002]. The RTM is run in scalar mode, simulating only the 1st element of the Stokes vector. The temperature dependence of the absorption by nitrogen dioxide (NO_2) and ozone (O_3) is included. Clouds below the field of view are neglected. Aerosols are completely neglected in this algorithm. Five orders of scattering are calculated.

Inversion procedure

The inversion procedure follows Sioris *et al.* [2004] and references therein. Chahine's method is used for the first iteration. Subsequent guesses rely on linear extrapolation or interpolation using the local Jacobian, $dSCD_{TH}/dx_{z=TH}$, where SCD is the BrO slant column density at a tangent height (TH) and x is the BrO number density at the tangent altitude. Slant column densities are determined from the measured and simulated radiances using an I_0 (reference spectrum) near TH=40 km.

Auxiliary data

Currently, the algorithm does not automatically calculate the TH offset or find cloud top height. These are found first with separate algorithms and stored values of TH offsets and cloud top height serve as input into the BrO profile retrieval. All other auxiliary data comes from the model. The ozone profile assumed in the forward modeling can be supplied from SCIAMACHY profile retrievals from limb scattering. The O_3 profile from the same limb scan is used. This option is generally preferred over O_3 profiles stored in the RTM's database of atmospheres.

Sensitivity and error analysis

The sensitivity and error analysis is summarized in Table 1. These retrieval errors arise from errors in the forward model or its inputs. Many of the inputs are geophysical (such as surface albedo, temperature profile, etc.). The error due to using only five orders of scattering is <1%. The error due to neglect of refraction leads to errors of ~0.5% or less in BrO slant column density and thus should be minor with respect to the retrieved BrO profile. The number of solar zenith angles (SZAs) around the limb in the line-of-sight direction is set to 21. The difference between 19 and 21 is minor (within convergence criteria), so this is also expected to be a minor error source.

A major source of systematic error comes from pointing. Using the ~305 nm knee, pointing accuracy is expected to be of the order of 300 m. This leads to errors of ~11% in the lower stratosphere and 5% errors at the top of the profile (30 km) of the opposite sign. The errors are expected to be smaller than this in the middle of the profile and the error in the BrO vertical column density (VCD) is ~1%.

For SZAs larger than 83°, the photochemical variation of BrO along the line-of-sight and in the incoming solar radiation is included in the RTM simulations. The error from neglecting the diurnal variation along the line-of-sight and in the incoming solar beam for SZA<83° is <10%.

There are also calibration problems and random errors from measurement noise. A typical wavelength shift of ~0.003 nm in the measured radiance relative to the absorber cross-sections results in a <3% error in BrO.

Table 1- Retrieval sensitivity to model simplifications and geophysical parameters used as model inputs. "T-dep" refers to the use of a coarse (20 K) temperature increment in the cross-section database.

				Impact on BrO	
Variable	**geometry**	**Control**	**Perturbed**	**Profile**	**VCD (>12 km)**
strat aerosol	SZA=60°, dϕ=90°	No aerosol	3% strat OD	1-2%	1-2%
O_3	SZA=54°, dϕ=59°	Mar 45° N	-10% (uniform)	≤2% (typical)	0.6%
NO_2	SZA=54°, dϕ=59°	Mar 45° N	-20% (uniform)	≤0.2% (typical)	<0.2%
air	SZA=80°, dϕ=149°	Mar 75° N	-2% (uniform)	≤2% (typical)	1.6%
BrO above	SZA=60°, 89°	MISU model	+30% (uniform)	0.1, 0.5% resp.	<0.5%
BrO below	SZA=33°	MISU model	+2.5e13/cm^2 (tropVCD)[1]	<1%	<1%

surf albedo	SZA=45º	18%	28%	<1%	<1%
T-dep	SZA=80º, dϕ=149º	231 K	fit w/ 221 K O_3	13.5% (30 km), 3% (12 km)	5%
T (systematic)	SZA=59º, dϕ=64º	Mar 45º N	+3 K	6% (30 km), 2% (12 km)	2%
T (random)	SZA=59º, dϕ=64º	Mar 45º N	±3 K	<2%	<2%
polarization	SZA=33º, dϕ:50,130º	I, Q, U	I (of Stokes vector)	<0.5% (worst at 12 km)	<0.2%

[1] assumes 1-km thick marine boundary layer containing 1.75×10^8 molec/cm^3 [Dickerson *et al.*, 1999]

Algorithm validation

The BrO profiles retrieved from this algorithm have been compared to those measured during by coincident balloon-borne instruments (SAOZ-BrO and LPMA). The profile comparisons are shown below in Figure 1 and 2. Additional validation material can be found in Dorf *et al.* [2006], including a comparison with the HALOX instrument on the Triple balloon.

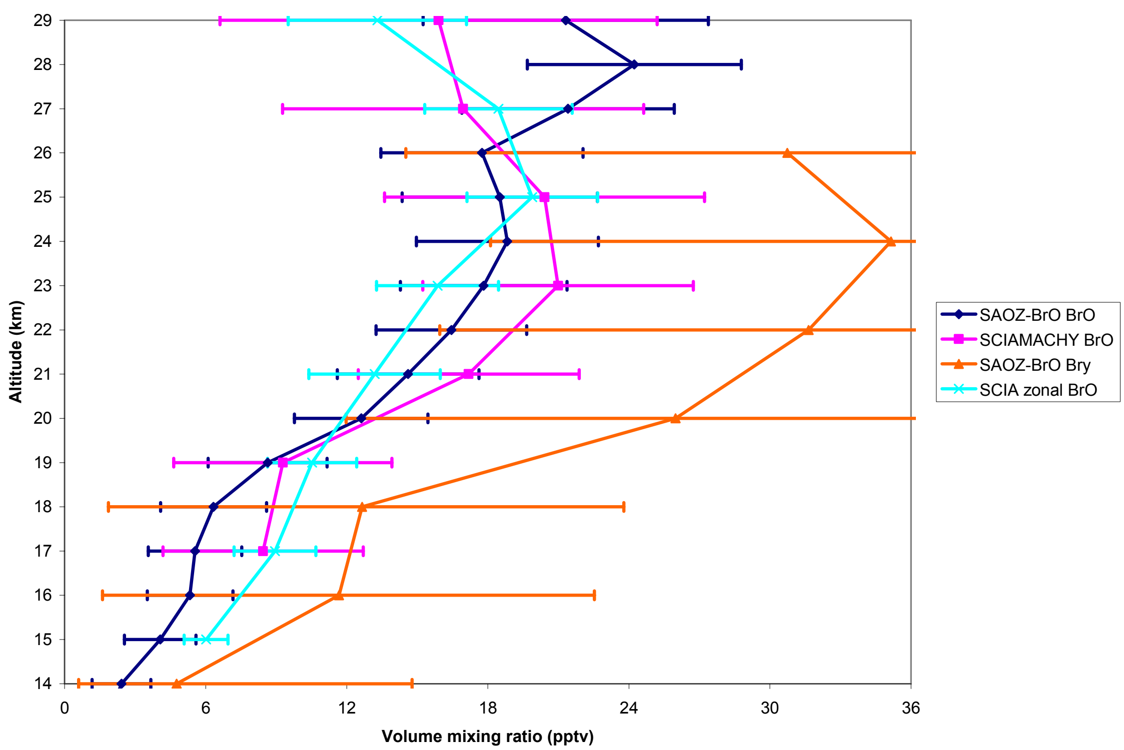

Figure 1- Coincident profiles of BrO from SCIAMACHY (44.7° N, 5° E) and SAOZ-BrO (43.8° N, 0.1° W) on 1 Oct. 2002, near Aire sur l'Adour, France. The SAOZ-BrO

BrO profile and its error bars, measured during evening ascent, were scaled to SCIAMACHY local time (~10 am, SZA=51°) using a photochemical model that was constrained by the SAOZ-BrO BrO and SAOZ NO_2 and O_3. The Br_y resulting from this constraint is also shown.

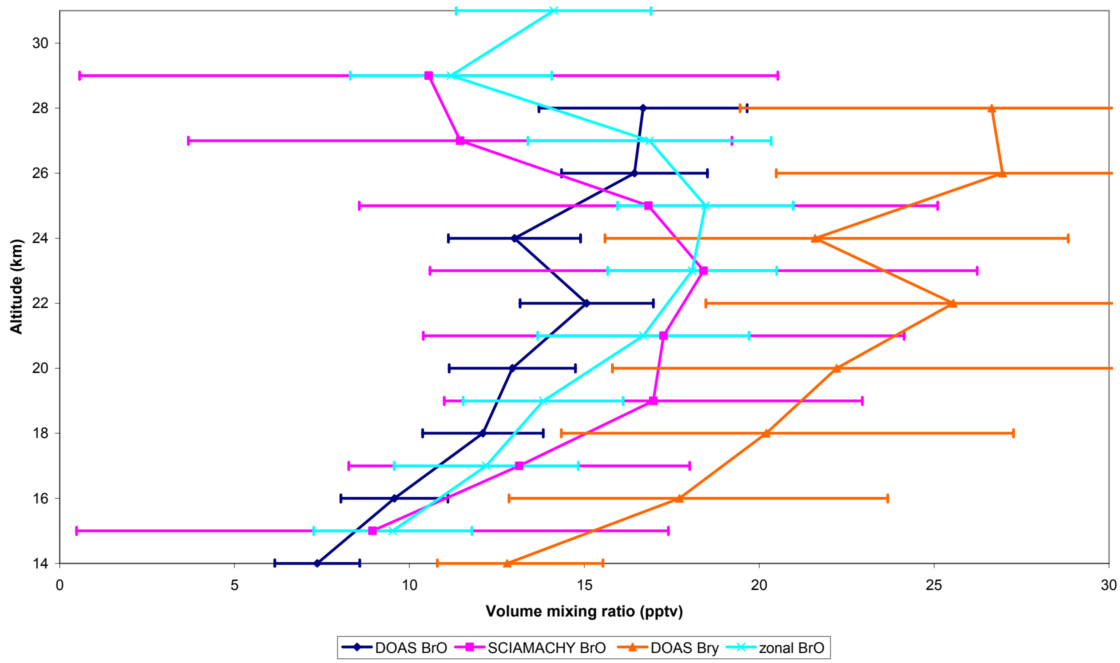

Figure 2- Coincidence between SCIAMACHY (64.5° N, 23.4° E) and LPMA/DOAS (67.9° N, 21.1° E) near Kiruna, Sweden on 23 March 2003. Profile observed by the balloon-borne DOAS during evening ascent was converted to SCIAMACHY local time (~11 am, SZA=64.4°). Also shown is the Br_y inferred from the DOAS instrument using the method described above assuming a scene albedo of 0.46, based on near-simultaneous satellite-nadir observations.

Recommendations for product validation

Product validation should use collocated NO_2 profile measurements to constrain diurnal scaling from SCIAMACHY local time to balloon local time. Profile measurements in the Antarctic vortex are recommended.

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