Algorithm description document for retrieval of SCIAMACHY vertical tropospheric NO_2 columns

Akhila Padmanabhan[1]
Randall V. Martin[1,2,3]
Aaron van Donkelaar[2]
Christopher E. Sioris[4]
Kelly V. Chance[3]
Thomas P. Kurosu[3]

[1]*Department of Chemistry, Dalhousie University, Halifax, NS, Canada*
[2]*Department of Physics and Atmospheric Sciences, Dalhousie University, Halifax, NS, Canada*
[3]*Harvard-Smithsonian Centre for Astrophysics, Cambridge, MA, USA*
[4] *Experimental Studies (ARQX), Air Quality Research Division, Environment Canada, Downsview, Ontario, Canada*

1. Introduction

Nitrogen Oxides (NO + NO_2), or NO_x, play an important role in climate change and air quality. NO_x largely controls tropospheric ozone production. NO_x oxidizes to nitric acid which impacts cloud properties and aerosol formation. Information from satellites provide a 'top-down' constraint for NO_x emissions.

2. Forward Model and Inversion Procedure

Following *Chance* [1998] and *Martin et al* [2002], we determine total slant columns of NO_2 by directly fitting backscattered radiance spectra from SCIAMACHY within the wavelength range of 429-452 nm, using measured reference spectra as described in section 3.

We remove the stratospheric column by first assuming that NO_2 over the central Pacific is primarily stratospheric and then subtracting the corresponding columns from the SCIAMACHY observations for the appropriate latitude and month. The resulting tropospheric columns are then corrected for the small amount of NO_2 over the Pacific using NO_2 columns obtained from GEOS-Chem simulations [*Martin et al*., 2006, www.geos-chem.org].

An air mass factor calculation is used to convert the tropospheric slant columns into vertical columns. This formula for the AMF follows *Palmer et al.* [2001]:

$$AMF = AMF_G \int_0^{\infty} w(z)S(z)dz \quad (1)$$

where AMF_G is the geometric AMF, w is the scattering weight, and S is the shape factor. The geometric AMF takes into account the geometry of the sun, satellite and earth and is a function of the solar zenith angle and satellite viewing angle. The scattering weights refer to the instrument's sensitivity to the trace gas as a function of altitude. We use the Linearized Discrete

Ordinate Radiative Transfer (LIDORT) model to calculate the scattering weights [*Spurr,* 2002]. The shape factor refers to the relative vertical distribution of NO_2 in the troposphere and is obtained from the GEOS-Chem chemical transport model. Monthly varying surface reflectivity fields are from *Kleipool et al.* [2008]. The aerosol correction uses daily local aerosol profiles obtained from a GEOS-Chem simulation of that scene [*Martin et al.,* 2003]. The AMF cloud correction depends on cloud fraction (what percentage of the observed scene is cloud-free), optical depth, and cloud height. The Fast Retrieval Scheme for Cloud Observables (FRESCO+) algorithm is used to correct for clouds[*Wang et al.,* 2008]. The vertical tropospheric NO_2 columns are obtained using the following calculation:

$$tropospheric\ vertical\ column = \frac{tropospheric\ slant\ column}{AMF}$$

3. Auxiliary Data needed

Spectral Fitting:	
NO_2 at 243K	*Bogumil et al.,* 2003
ozone at 223K	*Bogumil et al.,* 2003
H_2O at 296K	*Rothman et al.,* 1998
O_2-O_2 at 296K	*Rothman et al.,* 1998
Ring effect	*Chance and Spurr,* 1997
solar reference spectrum	*Chance and Kurucz,* 2010
AMF Calculation:	
cloud-top pressure	*Wang et al., 2008*
cloud fraction	*Wang et al., 2008*
surface reflectivity fields	*Kleipool et al*. 2008
NO_2 shape profiles	*GEOS-Chem*
aerosol correction	*GEOS-Chem*

4. Sensitivity and Error Analysis

The typical 1-sigma uncertainty for each SCIAMACHY measurement is estimated to be 40% due to the AMF plus 1×10^{15} molecules cm^{-2} caused by spectral fitting and subtraction of the stratospheric NO_2 column. The estimate for monthly mean uncertainty is $\pm(5 \times 10^{14}$ molecules $cm^{-2} + 30\%)$ which could include systematic errors [*Martin et al.,* 2006].

5. Algorithm Validation

As described in *Martin et al.* [2006], the tropospheric NO_2 columns were validated with coincident *in situ* measurements taken from the NASA DC-8 and the NOAA WP-3D aircraft as part of the ICARTT campaign. The two measurement techniques were consistent within their uncertainty. The retrieved columns tended to be lower than the columns derived from the *in situ* measurements in regions of enhanced NO_2 and higher in remote areas. The *in situ* measurements were also used to evaluate the GEOS-Chem simulated NO_2 vertical profiles used in the air mass factor formulation. Additionally, the GEOS-Chem vertical profiles were evaluated over the southeastern United States using aircraft measurements from TexAQS and SOS campaigns. Comparison of the AMFs calculated from the model profiles to those obtained from the *in situ* profiles generally showed agreement within a few percent *[Martin et al.*, 2004].

6. Recommendations for product validation

Martin et al. [2004] contains recommendations on the use of *in situ* measurements complemented with ground based observations. Vertically resolved measurements are needed that span the entire troposphere and are coincident in time and space with satellite overpasses. Validation should extend over large spatial regions over extended periods of time.

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