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Effect of temperature-dependent cross sections on O_4 slant column density estimation by a space-borne UV–visible hyperspectral sensor

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HIGHLIGHTS

- Temperature(T)-dependent cross section is used for O_4 slant column density (SCD).
- Effect of T-dependent cross section is significant for all satellite geometries.
- T-dependent cross section corrects difference of SCD between model and satellite.

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ABSTRACT

The sensitivities of oxygen dimer (O_4) slant column densities (SCDs) were examined by applying temperature-dependent O_4 cross sections using the radiative transfer model (RTM) calculation with the linearized pseudo-spherical vector discrete ordinate radiative transfer model. For the sensitivity study, we used a newly developed cross section database in place of the database used in the operational algorithm. Newly investigated O_4 cross section databases for 203 K and 293 K were used for the radiance simulation by interpolating temperature for each atmospheric layer based on the vertical profile of standard atmosphere in the RTM. The effect of the temperature-dependent cross sections was a significant O_4 SCD increase of 8.3% with dependence on satellite and solar viewing geometries. Furthermore, the O_4 SCD generally increased by an estimated 3.9% based on the observation geometries of the Ozone Monitoring Instrument. For the long-term comparison, the O_4 SCD estimated from the temperature-dependent cross sections corrects 20% of the total underestimation of O_4 SCD between the observation and simulation. Although the surface pressure variation and background aerosol effect also correct the O_4 SCD discrepancy, the effect of temperature-dependent cross sections was more important than the effects of surface pressure variation and background aerosols. Therefore, temperature dependence of the cross section in the RTM calculation is essential for the accurate simulation of O_4 SCD.

1. Introduction

Since the ability to measure atmospheric ozone using optical instruments was first achieved (Dobson and Harrison, 1926), the importance of spectroscopic techniques for measurements of atmospheric trace gases has increased. The differential optical absorption spectroscopy (DOAS) technique is a main method for retrieving trace gas concentrations by estimating slant column densities (SCDs) (e.g., Platt, 1994; Stutz and Platt, 1996; Wagner et al., 2007, 2010). For accurate estimation of vertical column densities (VCDs) and profiles of trace gases by the DOAS technique, the air mass factor (AMF) was introduced to convert SCDs to VCDs of trace gases (e.g., Noxon, 1975; Marquard et al., 2000; Lee et al., 2009a,b). Furthermore, the AMF calculation is customized depending on the trace gas species, such as NO_2 (e.g., Sarkissian et al., 1995; Boersma et al., 2004; Castellanos et al., 2015; Chimot et al., 2016), SO_2 (e.g., Lee et al., 2009a,b; Fioletov et al., 2011), HCHO (e.g., Chance et al., 2000; Palmer et al., 2001), and O_3 (e.g., Solomon et al., 1987; Veefkind et al., 2006), with consideration of the dependence on wavelength and regional characteristics of trace gas profiles.

The absorption band of oxygen dimer (O_4) is generated by collision-induced absorption of oxygens (O_2) (Pfeilsticker et al.,

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1997; Sneep et al., 2006; Thalman and Volkamer, 2013), and the absorption intensity is related to the square of the O_2 number concentrations due to absorption characteristics (e.g., Wagner et al., 2002; Hermans et al., 2003). Because atmospheric profiles of O_4 from O_2 are established and consistent, variation of O_4 absorption intensity is easily converted to the optical path length, and can be further utilized to obtain information on aerosols (Wagner et al., 2004, 2010), clouds (e.g., Accarreta et al., 2004; Sneep et al., 2008), and the AMFs of trace gases retrieved from the visible wavelength (e.g., Irie et al., 2008, 2011; Lee et al., 2009a,b, 2011; Clémer et al., 2010). Therefore, O_4 SCD estimation is important for the accuracy of trace gas retrievals. Because of the high sensitivity of O_4 SCDs to scattering properties of atmospheric particles, such as cloud and aerosol, the O_4 SCD from the DOAS method has also been employed in aerosol retrievals on ground-based (e.g., Wagner et al., 2004; Sinreich et al., 2005; Friess et al., 2006; Irie et al., 2008, 2011; Lee et al., 2009a,b, 2011; Clémer et al., 2010) and space-borne measurements [e.g., the Ozone Monitoring Instrument (OMI), Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, and Global Ozone Monitoring Experiment] in several observation studies (e.g., Wagner et al., 2010; Park et al., 2016).

Although several previous studies investigated and developed the database of temperature-dependent databases of O_4 cross sections (e.g., Greenblatt et al., 1990; Newnham and Ballard, 1998; Thalman and Volkamer, 2013), radiance simulation for O_4 SCD estimation has used temperature-independent absorption cross sections by assuming the effective temperature in the atmosphere (Accarreta et al., 2004; Clémer et al., 2010; Irie et al., 2011, 2015). However, retrieved O_4 SCDs have large discrepancies between model-based and observed radiance. For this reason, a scaling factor was investigated to compensate for a bias in SCDs derived from DOAS fitting due to cross section uncertainty. Empirically derived correction factors range from 1.20 to 1.40 for the differential O_4 SCD in ground-based measurements (Zieger et al., 2011; Clémer et al., 2010; Irie et al., 2011; Lee et al., 2011). To supplement the O_4 cross section database, Irie et al. (2015) empirically derived the correction factor (f_{O4}) by considering the elevation angle dependence. The main purpose of this elevation angle-dependent f_{O4} is to diminish the elevation angle dependence of the differential SCD for better retrieval results of the surface aerosol extinction coefficient and aerosol optical depth (AOD) from multi-axis DOAS (MAX-DOAS) measurements. The elevation angle dependence of f_{O4} is related to the change of effective temperature for observation (Irie et al., 2015; Spinel et al., 2015), but this issue is still under discussion in the observation community.

For satellite observations, Park et al. (2016) showed that the O_4 SCD from the radiative transfer model (RTM) exhibits a ratio of 0.86 ± 0.05 to the values from the OMI standard products over a clear-sky ocean surface. Although the RTM assumed to be 0.05 as ocean surface albedo, the O_4 SCD from the RTM underestimated 14% compared to the O_4 SCD from OMI standard product. To correct the discrepancy in O_4 SCDs between the model and observation, the assumed surface albedo was corrected to 0.10, which is a common ocean surface albedo value, instead of the climatological Lambertian equivalent reflectance (LER) for radiative transfer calculation (Park et al., 2016). After increasing the assumed surface albedo, the ratio was improved to 0.98 ± 0.05. However, there was positive (negative) bias in the large (small) O_4 SCDs, although assumed surface albedo was increased to double the common LER value of 0.05. On the other hand, the O_4 SCD discrepancy due to the different inversion methods, such as changing spectral window for DOAS analysis, is negligible if both SCDs are estimated to be the same radiance from the observation. For this reason, the discrepancy in O_4 SCDs between models and satellite observations is thought to be resolved by adopting multiple cross section datasets as a function of temperature, similar to the ground-based measurement.

In this study, the SCD calculation adopting temperature-dependent O_4 cross sections was examined to compare the SCDs from models and observations, and estimating the effect of temperature-dependent O_4 cross section for the model-based O_4 SCD calculations. The effect of temperature-dependent absorption cross sections for RTM calculation was quantified by performing a long-term comparison over a clear-sky ocean surface. By comparing the O_4 SCD from the model and observation, this study would to confirm the quantified correction due to temperature-dependent cross section effect for O_4 SCD discrepancy between model and observation. Section 2 explains the observation data of the OMI and the method for the O_4 SCD estimation from the radiance simulation. Section 3 presents the effect of the temperature-dependent cross section database on the O_4 SCD estimation, and a comparison between simulated O_4 SCDs and observations. Finally, the results and implications are summarized and discussed in Section 4.

2. Methods

The O_4 absorption bands are mainly located in the UV and visible range at 340, 360, 380, 446, 477, 532, and 630 nm (e.g., Greenblatt et al., 1990; Hermans et al., 1999; Thalman and Volkamer, 2013). In this study, the O_4 band at 477 nm was used to determine the O_4 SCD because the OMI has observed the O_4 SCD at 477 nm since 2004 to retrieve cloud information such as the radiative cloud fraction and effective cloud height. The OMI/Aura Level 2 cloud standard product (OMCLDO2) (e.g., Accarreta et al., 2004; Sneep et al., 2008) was used as the observed data for the comparison. To compare simulated and observed O_4 SCDs, the hyperspectral radiance was simulated from the RTM with different cross section databases.

2.1. OMI

The O_4 SCD in the OMCLDO2 was used as a representative dataset for O_4 SCD from satellite observation. The OMI channels are composed of two UV channels (UV-1: 270–314 nm, UV-2: 306–380 nm) and one visible channel (365–500 nm) (Levelt et al., 2006). The OMCLDO2 is retrieved by the visible channel [spectral resolution: 0.63 nm for full width at half maximum (FWHM)]. The spatial resolution is 13×24 km^2 at nadir view. The OMCLDO2 initially used the cross section database from Newnham and Ballard (1998). To consider temperature variation, the O_4 cross section is interpolated to 253 K for O_4 SCD in the OMCLDO2 (Accarreta et al., 2004). Recently, the O_4 absorption cross section was replaced with the database from Hermans et al. (1999) for the OMCLDO2 product (Sneep et al., 2008).

The DOAS method estimates the SCDs of trace gases with fitting errors converted from the residual spectrum. For this reason, inaccurate spectral information and large noise from the sensor decrease the accuracy of SCDs with increasing fitting errors. In this study, the precision of the O_4 SCD fitting from the OMI (Variable field name: Slant Column Amount O2O2 Precision) was selected as a fitting accuracy parameter, and the pixels of fitting precision less than 2% are selected for the analysis to minimize the effect of DOAS fitting error from the observed radiance. In addition, the quality flag (QF) parameters in the OMCLDO2 product, “Ground pixel quality flag,” “Xtrack quality flag,” “Measurement quality flag,” and “Processing quality flag,” were used to consider the measurement conditions. Because the main purpose of the OMCLDO2 is cloud information retrieval, the dataset simultaneously includes the cloud fraction (CF) in each pixel. For this reason, a CF value < 0.01 is applied as an index for distinguishing non-cloud pixels. The OMCLDO2 data were used for the period from 2005 to 2008 for the