Geophysical Research Abstracts Vol. 21, EGU2019-6680, 2019 EGU General Assembly 2019 © Author(s) 2019. CC Attribution 4.0 license.



Development of Hybrid algorithm based on DOAS and PCA for PBL SO₂ column retrieval from UV Hyperspectral satellite sensor

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In this study, we investigated the effects of signal-to-noise ration (SNR), ozone, aerosol, and measurement geometry on the PBL sulfur dioxide (SO₂) slant column density (SCD) retrieval accuracy using a Differential Optical Absorption Spectroscopy (DOAS) and a Principal Components Analysis (PCA) algorithm based on synthetic radiances under various observation conditions. Synthetic radiances for various observation conditions were made using linearized pseudo-spherical scalar and vector discrete ordinate radiative transfer (VLIDORT). We, then, retrieved SO₂ SCDs using two algorithms and compared the retrieved SO₂ quantities against true SO₂ SCD used for the RTM as input data. Comparing between the SO₂ SCD retrieval accuracy using PCA and DOAS under three SNR senarios (720, 1440, and 2880), we could clearly find that the performance of PCA is slightly better for the level of low SO₂ than DOAS. In case of SO₂ vertical column density (VCD) less than 8 × 1015 molecules cm-2, the average absolute percentage difference (APD) between true SO₂ SCDs and those retrieved by DOAS (PCA) increase to 148.7% (132.1%) under SNR 720 condition. Errors in PBL SO₂ SCD retrieval using two algorithms tend to significantly increase with total O₃ VCD, aerosol opdical depth (AOD), and solar zenith angle (SZA) under low SO₂ condition. For the surface reflectance of 0.04, the uncertainties of SO₂ SCD retrieval using DOAS (84.9%) at low SO₂ levels are significantly larger than that using PCA (70.0%). This study is the first to quantify the effect of the clean sector on the PBL SO₂ SCD retrieval accuracy using PCA. The high AOD and O₃ VCD in the clean sector are found to lead to large uncertainties in SO₂ SCD retrieval using PCA. Given the merits of which DOAS and PCA retrieval tequinge, we developed a new DOAS - PCA hybrid algorithm in which the SO2 SCD result of the DOAS method is used as the initial SO₂ SCDs to select pixels in the clean sector as input to the PCA algorithm. It may be thought to reduce the SO₂ SCD retrieval error caused by using the SO₂-contaminated pixels as the clean sector pixels in PCA algorithm. The SO2 retrieval performance of our hybrid algorithm is also analyzed and discussed using Geostationary Environment Monitoring Sensor (GEMS) synthetic radiance and Ozone Monitoring Instrument (OMI) L1B data.