

Supplemental Information.

Version 2 Ozone Monitoring Instrument SO₂ Product (OMSO2 V2): New Anthropogenic SO₂ Vertical Column Density Dataset

Can Li^{1, 2}, Nickolay A. Krotkov², Peter J. T. Leonard^{3, 2}, Simon Carn⁴, Joanna Joiner², Robert J. D.
5 Spurr⁵, Alexander Vasilkov⁶

¹Earth System Science Interdisciplinary Center, University of Maryland, College Park, MD 20742, USA

²NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA

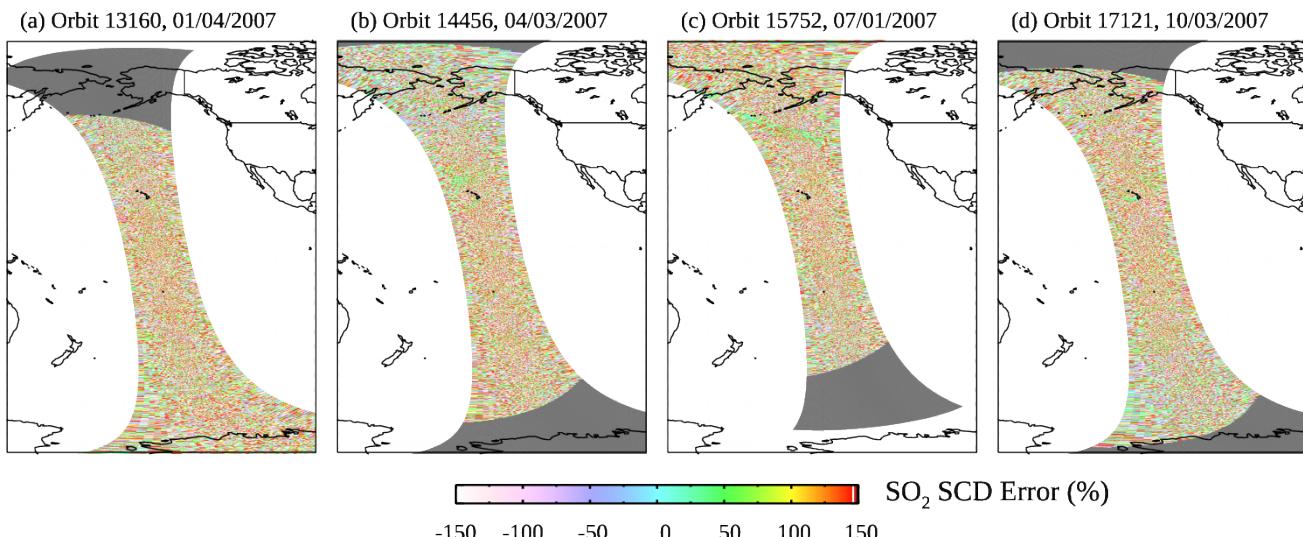
³ADNET Systems, Inc., Lanham, MD 20706, USA

⁴Michigan Technological University, Houghton, MI 49931, USA

10 ⁵RT Solutions Inc., Cambridge, MA 02138, USA

⁶Science Systems and Applications Inc., Lanham, MD, USA

Correspondence to: Can Li (can.li@nasa.gov)



15 Figure S1: The relative uncertainties in OMI SO₂ SCDs for the same four swaths as in Fig. 2, calculated as the ratio between the estimated uncertainty and the SCD for each pixel with SZA < 75°. The median relative uncertainty is ~30%, whereas the 5th, 10th, 25th, 75th, 90th and 95th percentiles are approximately -550%, -275%, -100%, 105%, 280% and 560%, respectively. Relative uncertainties for pixels with real SO₂ signals, for example, downwind of the Kilauea volcano in Hawaii are ~20-50%.

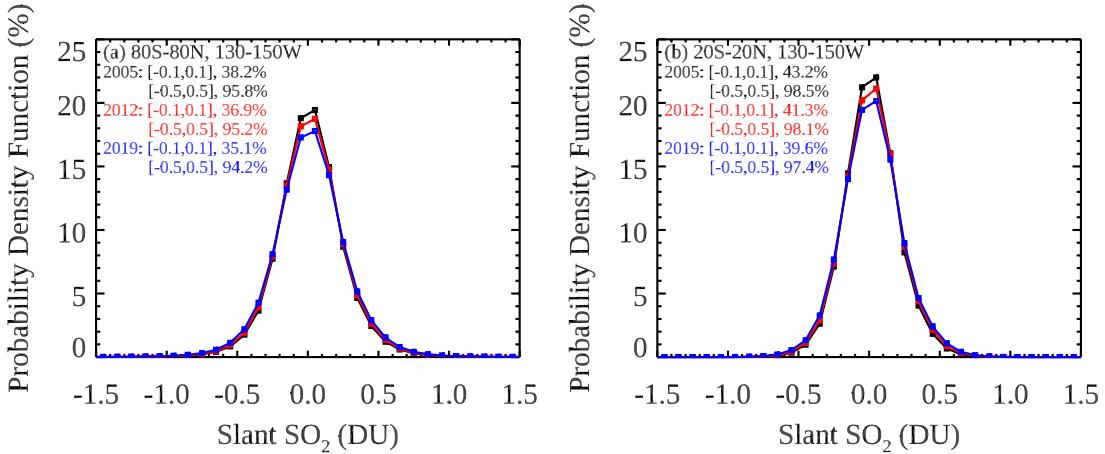


Figure S2: The probability density functions of OMI SO₂ SCDS over (a) the East Pacific and (b) the equatorial East Pacific for 2005 (black), 2012 (red) and 2019 (blue). The percentages of pixels that have SO₂ SCDS within the range of -0.1 to 0.1 DU and that of -0.5 to 0.5 DU for each year are also marked in the figure. Only pixels from rows 6-24 that are minimally affected by the row anomaly are included in the plots. Data from days potentially affected by large volcanic SO₂ plumes are also excluded.

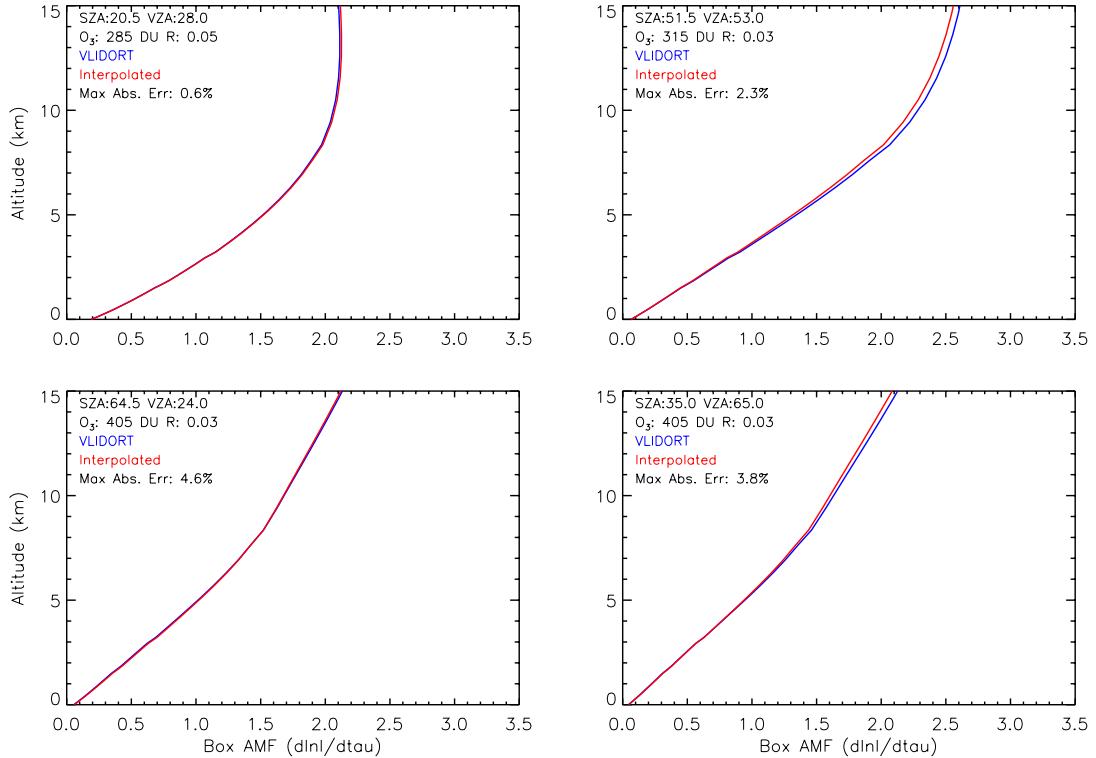
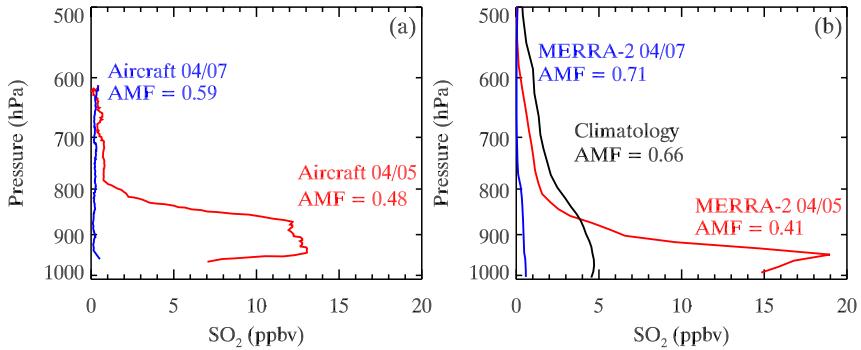
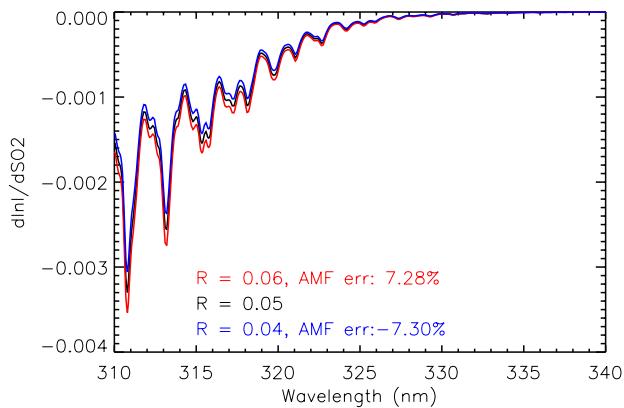


Figure S3: Profiles of box AMFs from VLIDORT direct calculations (blue) and box AMFs interpolated from precomputed lookup tables (red) for different O₃ profiles, SZAs and VZAs. All four cases here have surface reflectivity R = 0.03 or 0.05. Moreover, interpolation errors for these cases, defined as the relative differences between the interpolated and the directly calculated box AMFs, are generally < 10% at all levels between 0 and 15 km altitude. Cases with higher reflectivity (not shown) tend to have smaller interpolation errors.



30 Figure S4: (a) Aircraft-measured SO_2 profiles over a polluted area in northeastern China in April 2005 show large reductions in
30 SO_2 in just few days due to passage of a frontal system, leading to substantial changes in AMFs, calculated at 313 nm using the
measured profiles assuming $\text{SZA} = 30^\circ$, $\text{VZA} = 0^\circ$, $\text{RAA} = 90^\circ$, middle latitude O_3 and temperature profiles with $\Omega_{\text{O}_3} = 325 \text{ DU}$,
35 cloud fraction = 0, surface pressure = 1013.25 hPa and surface reflectivity $R = 0.05$. (b) AMF calculated using the monthly
climatology *a priori* profile over the same area for April (black) is biased high and does not reflect the day-to-day variation in (a).
AMFs calculated using daily model profiles (from MERRA-2, red for April 5, blue for April 7) better capture the effects of the
changing SO_2 profiles on AMFs.



40 Figure S5: SO_2 column Jacobians calculated assuming different values of surface reflectivity (R) indicating that an error of 0.01 in
 R would lead to about ~7% error in AMFs at 313 nm under these particular conditions. All calculations assume $\text{SZA} = 30^\circ$, $\text{VZA} =$
 0° , $\text{RAA} = 90^\circ$, middle latitude O_3 and temperature profiles with $\Omega_{\text{O}_3} = 325 \text{ DU}$, surface pressure = 1013.25 hPa, cloud fraction = 0,
and SO_2 mostly below 1 km.

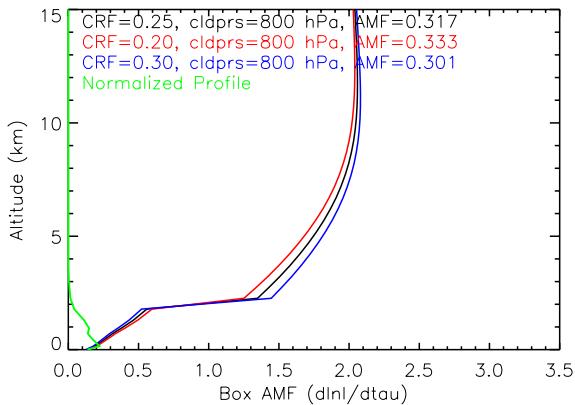


Figure S6: Profiles of box AMFs calculated assuming different cloud radiance fractions (CRF), cloud pressure = 800 hPa, SZA = 30°, VZA = 0°, RAA = 90°, middle latitude O₃ and temperature profiles with Ω_{O₃} = 325 DU, surface pressure = 1013.25 hPa, R = 0.05, and a PBL SO₂ profile (green line). An error of 0.05 in the cloud radiance fraction under these assumptions leads to ~5% error in AMF at 313 nm.

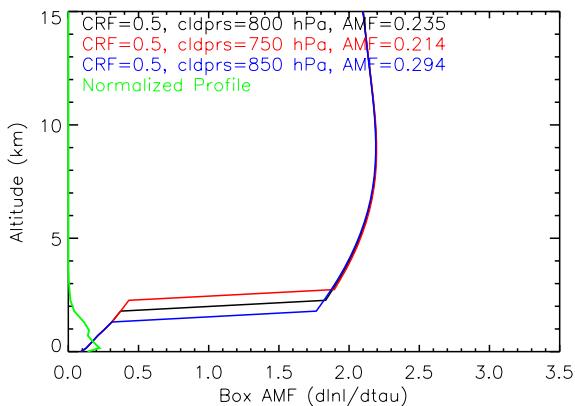


Figure S7: Profiles of box AMFs calculated assuming different cloud pressures, cloud radiance fraction = 0.5, and with the other conditions the same as those in Figure S6. Under these specifications, an error of 50 hPa in cloud pressure leads to up to ~25% error in AMF, while an error of 100 hPa leads to an error of almost 40%.

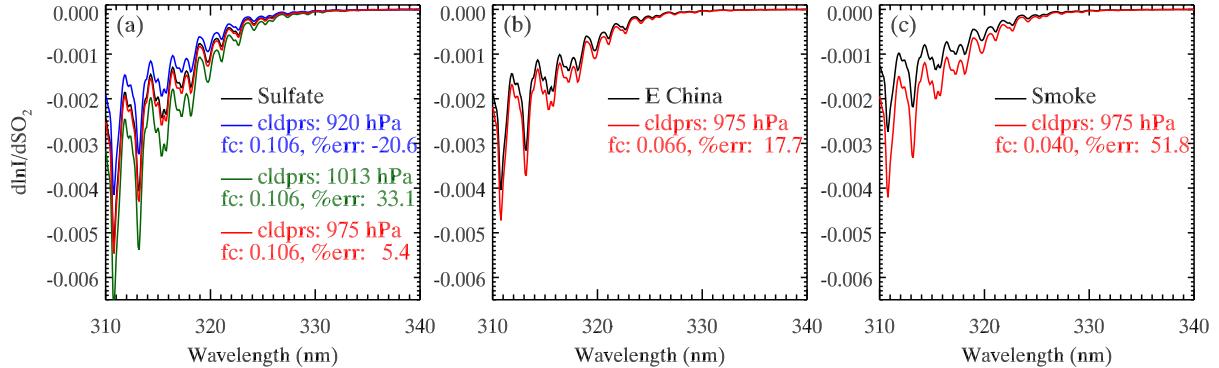


Figure S8: SO_2 Jacobians calculated with explicit corrections for the effects of (a) sulfate aerosols, (b) weakly absorbing industrial aerosols and (c) strongly absorbing smoke aerosols. For all types of aerosols, the same aerosol optical depth ($\text{AOD} = 1.0$ at 354 nm), size distribution (lognormal distribution with the effective radius, $r_{\text{eff}} = 0.1 \mu\text{m}$) and vertical distribution (an exponential profile with the scale height, $H = 0.9 \text{ km}$) are assumed, but the single scattering albedo is different ($\omega = 0.99, 0.95$ and 0.83 at 354 nm, respectively). All other assumptions are the same as those in Figure S5 with $R = 0.05$. Also plotted in coloured lines are SO_2 Jacobians estimated using the independent pixel approximation (IPA) approach to implicitly account for the aerosol effects. For the IPA estimates, an apparent effective cloud fraction is derived from the synthetic radiances with aerosols, assuming a cloud reflectivity of 0.8. A few different cloud/scene pressures are also assumed for scenarios with sulfate aerosols. The implicit aerosol correction in the IPA approach can lead to errors as large as 50% for smoke aerosols, with smaller errors for non-absorbing aerosols. Additionally, these errors have strong dependence on the vertical distributions of aerosols and SO_2 .