Supplement of Atmos. Meas. Tech., 13, 6175–6191, 2020
https://doi.org/10.5194/amt-13-6175-2020-supplement

Atmospheric Measurement Techniques
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Supplement of

Version 2 Ozone Monitoring Instrument SO_2 product (OMSO2 V2): new anthropogenic SO_2 vertical column density dataset

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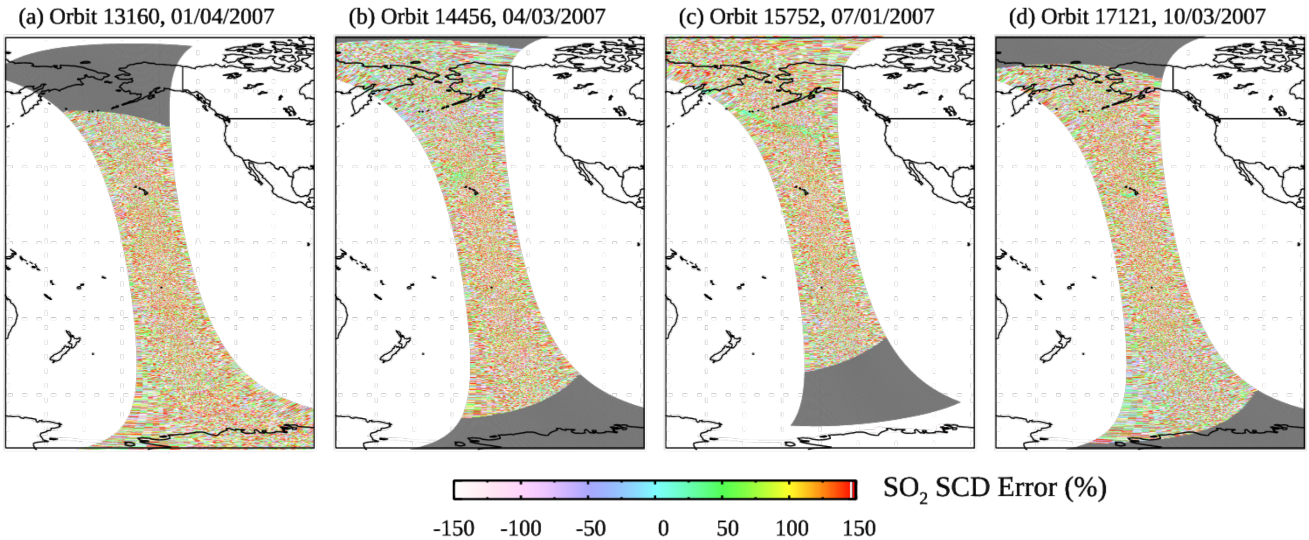

Figure S1: The relative uncertainties in OMI SO_2 SCDs for the same four swaths as in Fig. 2, calculated as the ratio between the estimated uncertainty and the SCD for each pixel with SZA < 75°. The median relative uncertainty is ~30%, whereas the 5th, 10th, 25th, 75th, 90th and 95th percentiles are approximately -550%, -275%, -100%, 105%, 280% and 560%, respectively. Relative uncertainties for pixels with real SO_2 signals, for example, downwind of the Kilauea volcano in Hawaii are ~20-50%.

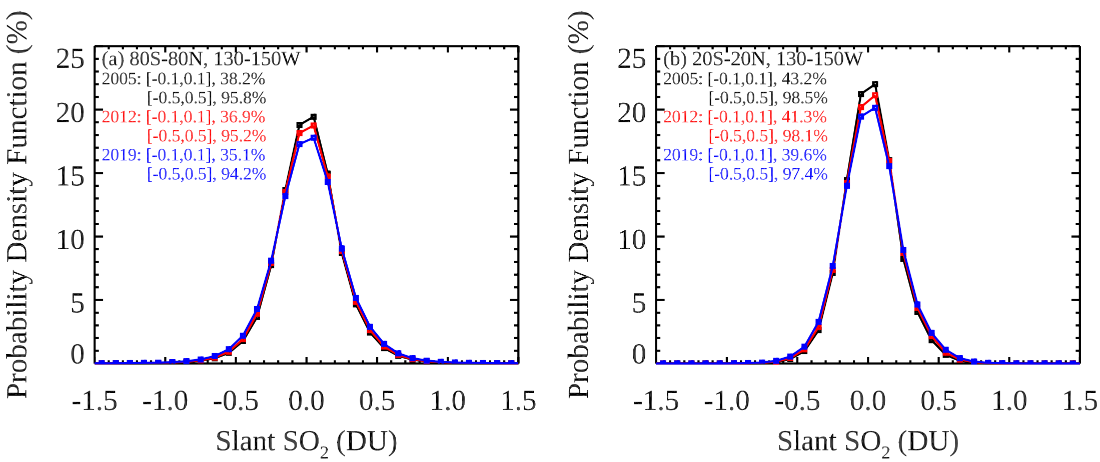

Figure S2: The probability density functions of OMI SO_2 SCDs over (a) the East Pacific and (b) the equatorial East Pacific for 2005 (black), 2012 (red) and 2019 (blue). The percentages of pixels that have SO_2 SCDs within the range of -0.1 to 0.1 DU and that of -0.5 to 0.5 DU for each year are also 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 SO_2 plumes are also excluded.

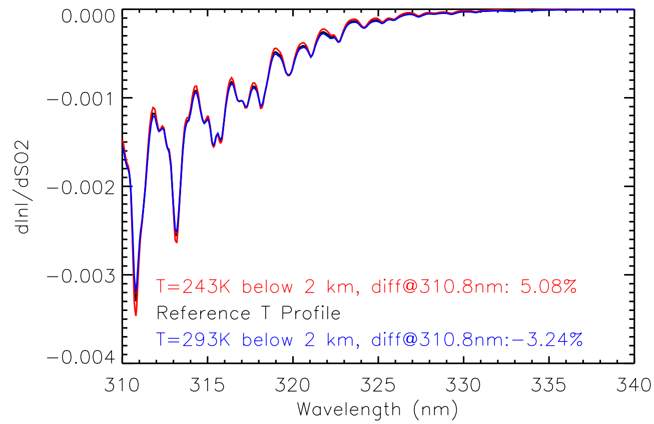

Figure S3: SO_2 column Jacobians calculated assuming different temperatures (T) for the lowest 2 km of the atmosphere. All calculations assume SZA = 30°, VZA = 0°, RAA = 90°, middle-latitude O_3 profile with Ω_{O3} = 325 DU, surface pressure = 1013.25 hPa, cloud fraction = 0, and SO_2 mostly below 1 km. The reference Jacobians (black) are used in OMSO2 V1.2 and 1.3 PBL SO_2 retrievals, assuming a temperature of ~284 K at the surface, decreasing to 270 K at 2 km. At 310.8 nm, the differences in Jacobians (reference - test case) are ~5.1% and -3.2% between the reference and test cases assuming constant temperatures of 243 K and 293 K below 2 km, respectively. The differences at 313 nm are 1.6% and -0.9% between the reference and the 243 K and 293 K cases, respectively.

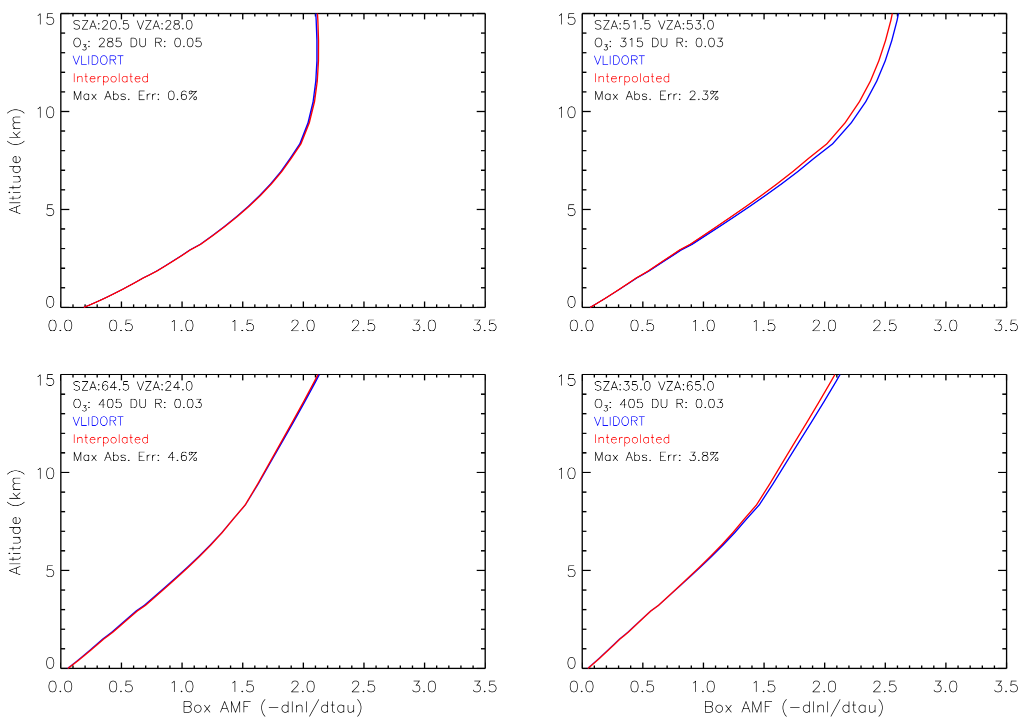

Figure S4: Profiles of box AMFs from VLIDORT direct calculations (blue) and box AMFs interpolated from precomputed lookup tables (red) for different O_3 profiles, SZAs and VZAs. All four cases here have surface reflectivity R = 0.03 or 0.05. Moreover, interpolation errors for these cases, defined as 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.

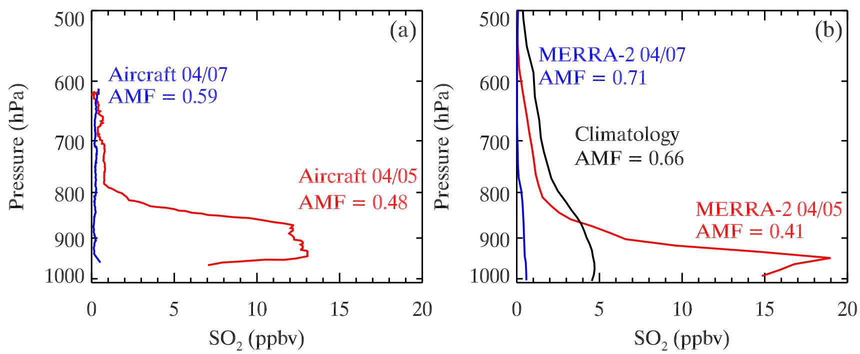

Figure S5: (a) Aircraft-measured SO_2 profiles over a polluted area in northeastern China in April 2005 show large reductions in SO_2 in just few days due to passage of a frontal system, leading to substantial changes in AMFs, calculated at 313 nm using the measured profiles assuming SZA = 30°, VZA = 0°, RAA = 90°, middle latitude O_3 and temperature profiles with Ω_{O3} = 325 DU, 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.

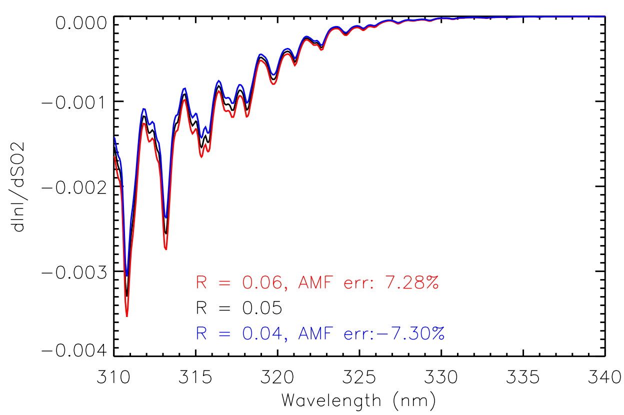

Figure S6: SO_2 column Jacobians calculated assuming different values of surface reflectivity (R) indicating that an error of 0.01 in R would lead to about ~7% error in AMFs at 313 nm under these particular conditions. All calculations assume SZA = 30°, VZA = 0°, RAA = 90°, middle latitude O_3 and temperature profiles with Ω_{O3} = 325 DU, surface pressure = 1013.25 hPa, cloud fraction = 0, and SO_2 mostly below 1 km.

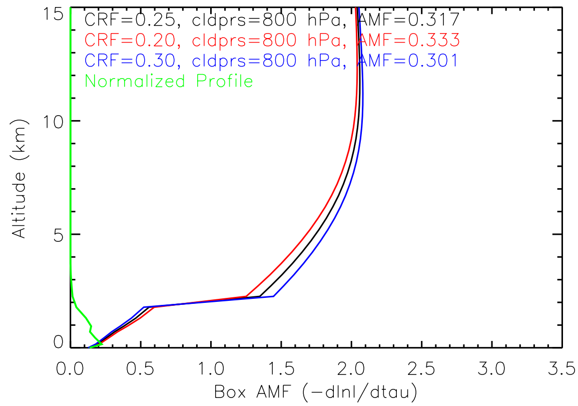

Figure S7: Profiles of box AMFs calculated assuming different cloud radiance fractions (CRF), cloud pressure = 800 hPa, SZA = 30°, VZA = 0°, RAA = 90°, middle latitude O_3 and temperature profiles with Ω_{O3} = 325 DU, surface pressure = 1013.25 hPa, R = 0.05, and a PBL SO_2 profile (green line). An error of 0.05 in the cloud radiance fraction under these assumptions leads to ~5% error in AMF at 313 nm.

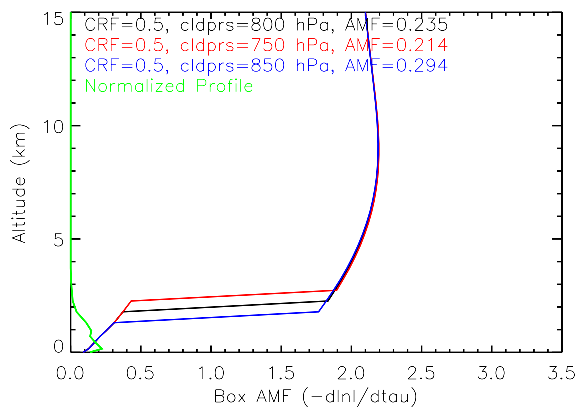

Figure S8: Profiles of box AMFs calculated assuming different cloud pressures, cloud radiance fraction = 0.5, and with the other conditions the same as those in Figure S6. Under these specifications, an error of 50 hPa in cloud pressure leads to up to ~25% error in AMF, while an error of 100 hPa leads to an error of almost 40%.

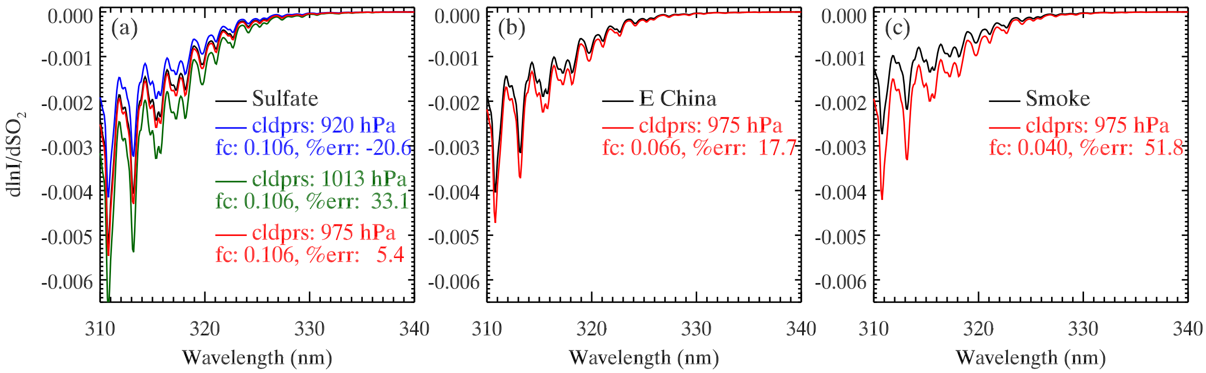

Figure S9: SO_2 Jacobians calculated with explicit corrections for the effects of (a) sulfate aerosols, (b) weakly absorbing industrial aerosols and (c) strongly absorbing smoke aerosols. For all types of aerosols, the same aerosol optical depth (AOD = 1.0 at 354 nm), size distribution (lognormal distribution with the effective radius, r_{eff} = 0.1 μm) and vertical distribution (an exponential profile with the scale height, H = 0.9 km) are assumed, but the single scattering albedo is different (ω = 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.