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Assessing the Ability of Satellites to Provide Air Quality Relevant Information: Analysis of DISCOVER-AQ Ozone and Precursor Data

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The NASA Earth Venture DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) project was designed to provide information for improving our ability to relate satellite observed column densities to surface mixing ratios of O_3, NO_2, and HCHO. DISCOVER-AQ combined P-3B aircraft in situ profiling of trace gas species, aircraft remote sensing of trace gas columns, observations of surface conditions from existing networks of air quality monitors, and remote sensing of trace gas columns from a network of ground-based Pandora UV/vis spectrometers collocated with air quality monitors. Here we consider data from the three warm-season DISCOVER-AQ field campaigns: Baltimore-Washington in July 2011; Houston, TX in September 2013; and the Front Range region of Colorado in July-August 2014. In the Maryland campaign lower tropospheric (0 to $\sim$5 km) O_3 columns derived from integration of P-3B profiles typically exhibited a statistically significant and high degree of correlation with surface data. These results suggest that O_3 partial column observations from future satellite instruments with sufficient sensitivity to the lower troposphere can be meaningful for surface air quality analysis. However, NO_2 columns typically exhibited a low to moderate degree of correlation with surface data. Distinct profile clusters emerged for the Texas and Colorado campaigns for O_3, indicating significant variability of O_3 profile shape. In contrast, very few distinct profile clusters emerged for NO_2 during any campaign, indicating the NO_2 profile behavior was relatively uniform throughout each campaign. The degree of vertical mixing (as indicated by temperature lapse rate) associated with each cluster exerted an important influence on the shapes of the median cluster profiles for O_3, as well as impacted the column vs. surface correlations for each cluster for both O_3 and NO_2. The CMAQ model reasonably captured the shape factor profiles for O_3 and NO_2 (better for O_3 than for NO_2), for the conditions associated with the Maryland campaign suggesting that a regional air quality models may adequately specify a priori profile shapes for use in remote sensing retrievals. We quantify spatial and temporal variability of both in-situ mixing ratios and column integrated O_3, NO_2, and HCHO during each deployment. Using structure function analyses, we compare simulated variability of output from the regional chemical models WRF/Chem and CMAQ with variability observed during the campaigns. Our analysis quantifies how often the atmosphere exhibits observationally relevant gradients in these key trace gas species, over what length scales they occur, and over what time periods. We compare both observed and simulated variability to the precision requirements for the forthcoming geostationary TEMPO instrument.