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Impact of high-resolution sea surface temperature, emission spikes and wind on simulated surface ozone in Houston, Texas during a high ozone episode

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Abstract

Model-measurement comparisons for surface ozone often show significant error, which could be attributed to problems in meteorology and emissions fields. A WRF-SMOKE-CMAQ air quality modeling system was used to investigate the contributions of these inputs. In this space, a base WRF run (BASE) and a WRF run initializing with NOAA GOES satellite sea surface temperature (SST) (SENS) were performed to clarify the impact of high-resolution SST on simulated surface ozone (O₃) over the Greater Houston area during 25 September 2013, corresponding to the high O₃ episode during the NASA DISCOVER-AQ Texas campaign. The SENS case showed reduced land-sea thermal contrast during early morning hours due to 1-2°C lower SST over water bodies. The lowered SST reduced the model wind speed and slowed the dilution rate. These changes led to a simulated downwind O₃ change of ~5 ppb near the area over land with peak simulated afternoon O₃. However, the SENS case still under-predicted surface O₃ in urban and industrial areas. Episodic flare emissions, dry sunny postfrontal stagnated conditions, and land-bay/sea breeze transitions could be the potential causes of the high O₃.

In order to investigate the additional sources of error, three sensitivity simulations were performed for the high ozone time period. These involved adjusted emissions, adjusted wind fields, and both adjusted emissions and winds. These scenarios were superimposed on the updated SST (SENS) case. Adjusting NO_x and VOC emissions using simulated/observed ratios improved correlation and index of agreement (IOA) for NO_x from 0.48 and 0.55 to 0.81 and 0.88 respectively, but still reported spatial misalignment of afternoon O₃ hotspots. Adjusting wind fields to represent morning weak westerly winds and afternoon converging zone significantly mitigated under-estimation of the observed O₃ peak. For example, simulations with adjusted

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