



Analysis of radicals, radical precursors and chemical transformations for Houston/Texas

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Air quality simulations were performed for the Houston-Galveston-Brazoria area for springtime conditions in May and June of 2009. Meteorological parameters predicted by Weather Research and Forecasting (WRF) model, for which data assimilation with recursive objective analysis was performed, are well simulated most of the time. The Community Multiscale Air Quality (CMAQ) model driven by meteorology from WRF simulates ozone and many other trace species, including radical precursors such as HCHO and HONO, with a satisfactory agreement with observations. While CMAQ satisfactorily captures the daily variations of the OH radical, it sometimes underestimates its high daytime values. Concentrations of HO₂ are often underpredicted in polluted air masses and persistently severely underpredicted at low NO_x conditions, when the Houston air is affected by marine air masses. In contrast, concentrations of H₂O₂ and CH₃OOH are almost always overpredicted by the model, the overprediction occurs frequently in the polluted air and occurs always when marine air is encountered. Those mispredictions are consistent despite day-to-day variations in meteorological conditions and emissions and bring into question current representation of radical-related chemistry in the model as radical production and recirculation in the model is overtaken by termination processes and creation of more stable compounds, such as H₂O₂ and CH₃OOH. Smaller model biases of H₂O₂ and peroxides are associated with lower humidity. The relative importance of various photolysis processes as radical sources in the Houston atmosphere was also elucidated. Morning HO_x formation is dominated by HONO while ozone contributes the most during midday. HONO contribution to HO_x formation is more pronounced at the surface layer where most of it is formed, radical production from ozone is more important at elevated levels where higher concentrations of ozone are observed. Formaldehyde contributes up to 40% and also peaks during midday, but on days when high morning concentrations of formaldehyde are observed, its contribution to HO_x in the morning exceeds that of ozone. Photolysis of H₂O₂ is a minor contributor to radical levels.