Large-eddy simulation of atmospheric chemistry during the DISCOVER-AQ 2011 campaign

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This research implements 2011 DISCOVER-AQ field campaign measurements in Baltimore-Washington, D.C. region in conjunction with the NCAR Large Eddy Simulation (LES) model to understand and improve simulations of the vertical distributions of key BVOC species. We categorize three distinct weather systems, including fair weather condition, convective precipitation event, and polluted event under high temperature. LES simulated potential temperature and water vapor mixing ratio match fairly well with P-3B observations under all the chosen weather cases. Higher temperature and larger water vapor mixing ratio induce stronger convection in the convective case and the high temperature case, and also lead to elevated concentrations of all the chemical species throughout the vertical profiles. LES generates realistic results for isoprene, and can capture the correct average concentration of O_3, while, NO and NO_2 are underestimated due to the assumption of low NOx emission. WRF NEI 2005 and 2011 emission inventories are compared, and NEI 2011 emissions will be used to update LES in our future work.