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Simulation of secondary organic aerosols over the Indian region using a global climate model with extensive interactive atmospheric chemistry

Pawan Vats (1), Dilip Ganguly (1), Vinayak Sinha (2), and Lokesh Sahu (3)

(1) Indian Institute of Technology, Delhi, Centre for Atmospheric Sciences, India (pawanvats5086@gmail.com), (2) Indian Institute of Science Education and Research, Mohali, Earth and Environmental Sciences Department, India (vsinha@iisermohali.ac.in), (3) Physical Research Laboratory, Ahmedabad, Space and Atmospheric Sciences Division, India (lokesh@prl.res.in)

Despite the large contributions of secondary organic aerosols (SOA) to fine particulate mass, most global climate models do not include SOA formation to avoid representation of complex physico-chemical processes governing SOA formation. In the present study, we evaluate the simulation of major aromatic secondary organic aerosols (ASOA), namely, benzene, toluene, and xylene by the Community Atmospheric Model version 4 with coupled extensive interactive atmospheric chemistry (CAM4-Chem) using in-situ observations available from selected locations in India. Comparison of simulated concentrations of aromatic volatile organic compounds (VOCs) with available in-situ observations over India suggests that the CAM4-Chem model underestimates VOC concentrations by up to a factor of 10 in some seasons. This underestimation of aromatic VOC concentrations by the CAM4-Chem model has serious implications for realistic predictions of various atmospheric pollutants such as tropospheric ozone (O_3) , NO_x , ASOA, and hence in the estimates of atmospheric radiative forcing over the Indian region by this model. There are some evidences which suggest that the underestimation of VOCs by the CAM4-Chem is at least in part due to underestimation of VOC emission inventories used in the model. We perform simulations of CAM4-Chem for a period of 5 years (2011-2015) in the "specified dynamics" mode, enabling us to constrain the model meteorology to match with the meteorological analysis from MERRA-2 by prescribing winds, temperature, surface heat and moisture fluxes, while aerosol mass concentration evolves according to the model's governing equations. As part of our sensitivity study, we perform five different simulations of CAM4-Chem, each one for the same period as mentioned earlier, however with (i) default model configuration, (ii) modified emissions of VOCs, (iii) modified emissions of nitrogen oxides (NO $_x$) over India, (iv) modified values of stoichiometric coefficients (SC), and (v) a combination of all three earlier modifications. In order to modify the VOC emissions over India, we used the results from in-situ measurements of aromatic VOCs available over Mohali and Udaipur. And satellite observations of OMI to modify the NO emissions over India and results from previous laboratory experiments for estimating SC to suitably modify SC values used in the model. The spatio-temporal variability of simulated concentrations of VOC and ASOA are compared with available measurements at selected locations in India. We find large variability in simulated concentrations of VOCs and ASOA over the Indo Gangetic Plain (IGP) region among various sensitivity simulations suggesting that the IGP is a hot spot region for VOCs and ASOA production. We further note that the variability in VOCs and ASOA concentrations are maximum during the months of October and November. Results from our sensitivity simulations suggests that a combination of modified emissions of VOC, NOx, and stoichiometric coefficients in the model yields VOC and ASOA concentrations closest to available observations over India. More results with greater details will be presented.

Keywords: Aromatic Secondary Organic Aerosols, Volatile Organic Compounds, Stoichiometric Coefficient, NO_x , CAM4-Chem model.