4.049 Evaluation of updated isoprene, terpene and aromatic oxidation in the MOZART chemical mechanism.

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Abstract:

Recent laboratory and field observations have provided important advances in our understanding of the oxidation pathways of isoprene and terpenes, which are the major natural contributors of volatile organic compounds (VOCs) to the atmosphere, and precursors to ozone and secondary organic aerosols (SOA). Intermediate isoprene oxidation products, such as isoprene epoxydiols (IEPOX), hydroperoxy aldehydes (HPALD), isoprene peroxides and isoprene nitrates, have been measured during several field campaigns in the Southeast United States. The MOZART tropospheric chemistry mechanism has been expanded to specifically represent these measured intermediate compounds, thus allowing for quantitative evaluation of the model representation of the emissions and chemical evolution of isoprene and terpenes. The MOZART chemistry has also been expanded to treat specific aromatic species (benzene, toluene, xylenes) instead of a single lumped aromatic compound. The NSF/NCAR/NASA DC3, NSF/NCAR NOMADSS, NASA SEAC4RS and NSF/NCAR FRAPPE aircraft campaigns provide simultaneous observations of numerous VOCs using several instruments and measurement techniques, such as TOGA (Trace Organic Gas Analyzer, fast GC-MS), WAS (whole air sampler), CIMS (chemical ionization mass spectroscopy) and PTR-MS (proton-transfer-reaction mass spectroscopy). The MOZART chemical mechanism is used in both a box model (BOXMOX) and the global chemistry climate model CAM-chem (Community Atmosphere Model with Chemistry, a component of the Community Earth System Model) for evaluation and comparison to previous chemistry schemes. BOXMOX is initialized using the field campaign observations for a variety of locations to evaluate the chemistry under a mixture of natural and urban conditions. CAM-chem is run with specified dynamics to represent the specific dates of the campaigns and allow direct comparison between model results and observations. CAM-chem includes online biogenic emissions using the MEGAN v2.1 algorithms, and the airborne measurements are used to evaluate

the biogenic emissions of isoprene, monoterpenes, methanol, acetone, acetaldehyde, and other compounds.