2.1 New chemistry and diagnostics for the MOZART chemistry suite in WRF-Chem.

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In WRF-Chem V4.0 the T1-MOZCART chemistry mechanism, which is an update of the MOZCART chemistry, has been added. The T1-MOZCART chemistry expands the isoprene oxidation scheme, splits lumped aromatics and terpenes into individual species, has a more detailed representation of organic nitrates, and includes heterogeneous reactions. The new chemistry allows for better evaluation of volatile organic compounds with observations. Preliminary analysis of one test case shows 2 ppbv difference in ozone over the western U.S. As part of the MOZART chemistry suite, we have updated Henry's Law coefficients, creating a table that can be accessed by wet deposition, dry deposition, and convective-parameterized wet deposition ensuring that these values are used consistently across the model. With the MOZART suite of chemistry options, we have implemented diagnostics to output integrated reaction rates during the simulation, allowing the user to find the important chemical reactions as well as determine characteristics such as ozone production efficiency. These new developments in WRF-Chem will be illustrated with simulations of case studies from the FRAPPÉ field experiment in Colorado and the SEAC4RS experiment in the southeast U.S. Our plans for future development with WRF-Chem and Multiscale Infrastructure for Chemistry and Aerosols will also be discussed.