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Improving the simulation of Intermediate Volatility Compounds (IVOCs) in chemical transport models

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Secondary organic aerosol (SOA) can be formed in the atmosphere through oxidation of volatile (VOCs), intermediate volatility (IVOCs) and semivolatile organic compounds (SVOCs), and condensation of their less volatile products to the particulate phase. While there has been a lot of progress with the simulation of the VOC chemistry, the simulation of the IVOCs remains challenging. In this study, we develop a new approach for the treatment of these compounds in chemical transport models, treating them as lumped species, similar to the VOCs. The new species are implemented in the SAPRC gas-phase chemical mechanism. We introduce four new lumped species representing larger alkanes, two species for polyaromatic hydrocarbons (PAHs) and one new lumped species representing aromatics, all in the IVOC volatility range. Their gas-phase chemistry is assumed to be analogous to that of the large alkanes and aromatics currently in the SAPRC mechanism but with appropriate parameters. The SOA yields for these additional species were estimated for low and high-NOx conditions following the Volatility Basis Set framework and using the available results of smog chamber studies. As most emission inventories do not include IVOCs, we estimated their emissions starting from road transport using existing non-methane hydrocarbons emissions and emission factors of individual IVOCs from laboratory studies. The total IVOC emissions from diesel vehicles for Europe were significantly higher than those coming from gasoline vehicles. The emissions and extended mechanism were implemented in PMCAMx and were used to simulate the EUCAARI intensive period. Cyclic alkanes, which have both high SOA yields and high emissions, were a major SOA precursor group. The contribution of the various IVOCs to SOA formation, and their overall role is discussed. Significant remaining uncertainties are summarized.