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VOC reactivity in central California: comparing an air quality model to ground-based measurements

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Abstract. Volatile organic compound (VOC) reactivity in central California is examined using a photochemical air quality model (the Community Multiscale Air Quality model; CMAQ) and ground-based measurements to evaluate the contribution of VOC to photochemical activity. We classify VOC into four categories: anthropogenic, biogenic, aldehyde, and other oxygenated VOC. Anthropogenic and biogenic VOC consist of primary emissions, while aldehydes and other oxygenated VOC include both primary anthropogenic emissions and secondary products from primary VOC oxidation. To evaluate the model treatment of VOC chemistry, we compare calculated and modeled OH and VOC reactivities using the following metrics: 1) cumulative distribution functions of NO_x concentration and VOC reactivity ($R_{OH,VOC}$), 2) the relationship between $R_{OH,VOC}$ and NO_x, 3) total OH reactivity ($R_{OH,total}$) and speciated contributions, and 4) the relationship between speciated $R_{OH,VOC}$ and NO_x. We find that the model predicts $R_{OH,total}$ to within 25–40% at three sites representing urban (Sacramento), suburban (Granite Bay) and rural (Blodgett Forest) chemistry. However in the urban area of Fresno, the model under predicts NO_x and VOC emissions by a factor of 2–3. At all locations the model is consistent with observations of the relative contributions of total VOC. In urban areas, anthropogenic and biogenic $R_{OH,VOC}$ are predicted fairly well over a range of NO_x conditions. In suburban and rural locations, anthropogenic and other oxygenated $R_{OH,VOC}$ relationships are reproduced, but calculated biogenic and aldehyde $R_{OH,VOC}$ are often poorly characterized by measurements, making evaluation of the model with available data unreliable. In central California, 30–50% of the modeled urban VOC reactivity is due to aldehydes and other oxygenated species, and the total oxygenated $R_{OH,VOC}$ is nearly equivalent to anthropogenic VOC reactivity. In rural vegetated regions, biogenic and aldehyde reactivity dominates. This indicates that more attention needs to be paid to the

accuracy of models and measurements of both primary emissions of oxygenated VOC and secondary production of oxygenates, especially formaldehyde and other aldehydes, and that a more comprehensive set of oxygenated VOC measurements is required to include all of the important contributions to atmospheric reactivity.

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