

Abstract

Although the yield for the formation of secondary organic aerosol (SOA) from the oxidation of isoprene is small relative to other compounds, it is important to understand this phenomenon because of the predominance of isoprene emissions on local, regional, and global scales. To that end, a zero-dimensional model that describes the gas-phase chemistry of isoprene and its daughter products and the thermodynamic phase partitioning of those products with low enough volatility to produce SOA has been developed. The gas-phase chemistry was developed in the framework of the Caltech Atmospheric Chemistry Mechanism, and the phase distribution was determined using a simplified version of the Model to Predict the Multi-phase Partitioning of Organics. Four scenarios were considered: a low-nitrogen oxide (NO_x) photochemical scenario, a high- NO_x photochemical scenario, a nitrate radical (NO_3) scenario, and a scenario in which the small dicarbonyls glyoxal (GLY) and methyl glyoxal (MGLY) were taken up assuming first-order rate constants determined from the literature. Regardless of scenario, it appears that the most important routes for SOA formation come from the phase partitioning of non-volatile products (likely dimers, trimers, etc.). However, the most important route of formation of these non-volatile products depended strongly on the scenario. In the low- NO_x case, oxidation of methacrolein (MCR) and epoxide products leads to these species. In the high- NO_x case, the MCR case was most dominant (because epoxides are less likely to form in the presence of NO_x). In the NO_3 case, organic peroxy radical self reactions formed the non-volatile SOA products. It is hypothesized that the MCR- NO_3 reaction also is important. For the simulation conditions chosen, the reactive uptake of GLY and MGLY is relatively less important than the formation of SOA from

thermodynamic partitioning of the non-volatile products.