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Evaluation of New Secondary Organic Aerosol (SOA) Models for a Case Study in Mexico City

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Recent field studies have found large discrepancies in the measured vs. modeled SOA mass loadings in both urban and regional polluted atmospheres. The reasons for these large differences are unclear. Here we revisit a case study of SOA formation in Mexico City described by Volkamer et al. (GRL, 2006) and show that the increase in OA/ΔCO during photochemistry is consistent with results from several groups during the MILAGRO 2006 campaign, and that the impact of regional primary biomass burning OA is minor or negligible. Then we use the case study to evaluate three new SOA models: the update of aromatic SOA yields from recent chamber experiments (Ng et al., ACP, 2007); the formation of SOA from glyoxal (Volkamer et al., GRL, 2007); and the formation of SOA from primary semivolatile and intermediate volatility species (P-S/IVOC) (Robinson et al., Science, 2007). We also evaluate the effect of reduced partitioning of SOA into POA (Song et al., GRL, 2007). Traditional SOA precursors (mainly aromatics) by themselves still fail to produce enough SOA to match the observations by a factor of 7. The new low-NOx aromatic pathways with very high SOA yields make a very small contribution in this urban environment as the RO_2 + NO reaction dominates the fate of the RO_2 radicals. Glyoxal contributes several μg m^{-3} to SOA formation, with similar timing as the measurements. P-S/IVOC are estimated from equilibrium with emitted POA, and introduce a large amount of carbon that was not in models before. With the formulation in Robinson et al. (2007) these species have a high SOA yield, and this mechanism can close the gap in SOA mass between measurements and models in our case study. However the volatility of model SOA produced is too high when compared to that measured using a thermal denuder, while the O/C ratio is lower than observations. The sensitivities of the model to some key uncertain parameters are evaluated.