1.140 Modeling and Constraining the Production and Composition of Secondary Organic Aerosol from a Diesel Engine using Parameterized and Semi-Explicit Chemistry and Thermodynamics Models.

Early Career Scientist

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Abstract:

Photochemistry experiments were performed with the potential aerosol mass (PAM) reactor at Colorado State University in the summer of 2015. The goal was to investigate primary emissions and secondary production of organic aerosol (OA) from a representative non-road diesel engine under varying engine load and fuel combinations. SOA production dominated POA emissions by an order of magnitude after 1.5 days of simulated atmospheric aging, idle loads produced the highest POA and SOA levels and biodiesel results were identical to those from diesel. In this work, we used two state-of-the-science frameworks, namely the volatility basis set (VBS) developed by Donahue and coworkers and the statistical oxidation model (SOM) developed by Cappa and coworkers to simulate the production and composition of SOA in those experiments. Leveraging recent laboratory-based inputs, both frameworks accounted for a semi-volatile and reactive POA, SOA production from volatile organic compounds (VOCs) and intermediate-volatility organic compounds (IVOCs), NO_X- dependent multigenerational gas-phase chemistry and dynamic gas/particle partitioning. Both model frameworks demonstrated that for model predictions of SOA mass and composition to agree with measurements across all engine load-fuel combinations, it was (a) quintessential to account for SOA formation from IVOCs (IVOCs were found to account for about three-quarters of the model-predicted SOA) and (b) necessary to dynamically model the gas/particle partitioning using a mass accommodation coefficient of approximately 0.1. Model predictions of the gas-phase organic compounds (resolved in carbon and oxygen space) from the SOM compared favorably to gas-phase measurements made using a Chemical Ionization Mass Spectrometer (CIMS). Qualitatively, this finding substantiates the semi-explicit chemistry captured by the SOM and the measurements made by the CIMS. Work is under way to examine the sensitivity of the findings to the use of alternate emissions profiles and treatment of vapor wall-losses.