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NESL's Atmospheric Chemistry Division Seminar

Simulating Secondary Organic Aerosol at Varying Levels of Complexity

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3:15 PM – Refreshments
3:30 PM – Seminar

FL2 1022- Large Auditorium

Abstract

Secondary organic aerosol (SOA) is a major component of sub-micron particulate mass. Despite intense focus over the past decade, regional air quality and climate models continue to do a relatively poor job of accurately simulating SOA concentrations, properties and spatial extent, typically underestimating observed concentrations. SOA formation within these models is highly parameterized and predominantly based on observed SOA yields from smog chamber experiments. SOA formation is actually a very complex process that involves hundreds (if not thousands) of individual species.

Models such as GECKO-A aim to capture this complexity through explicit simulation of the chemistry involved. The detailed information available from GECKO-A allows for insights into the key reactions and species involved to be developed, but is too complex for 3D models. The simplest models (used in 3D models) discard nearly all of the actual complexity, parameterizing SOA formation as involving just a handful of species. Although computationally efficient, the simplicity of these parameterizations makes it difficult to establish how well they can be extrapolated to the atmosphere- model/measurement comparisons thus far would suggest not well.

There is a need for the development of intermediate complexity models that aim to retain some essence of the fundamental chemistry that drives the oxidation and SOA formation process, but that are simple enough to be used on a more routine basis than chemically explicit models. I will discuss the development of one such model, the Statistical Oxidation Model (SOM). The SOM will be compared with results from GECKO-A to ascertain how well the explicit and intermediate complexity approaches agree, and the GECKO-A model output will be utilized to further refine the parameterizations inherent in the SOM. Finally, I will discuss how these models can be used to ascertain the extent to which typical smog chamber experiments are biased due to losses of gases onto the chamber walls.

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