Abstract: Secondary organic aerosols (SOA) account for a significant fraction of submicron aerosols. SOA formation changes the preexisting aerosol size distribution, which affects the aerosol direct and indirect radiative forcing, but currently there are no tools to simulate this evolution of aerosol size distribution. Here we developed a new moment-based parameterization scheme, MOMSOA, to describe the evolution of aerosol size distribution due to SOA formation. The scheme is highly computationally-efficient without losing detailed physicochemical information. We implemented MOMSOA into WRF-Chem model to improve the model ability to simulate SOA. From June 13th to June 21th, the model simulates aging of SOA precursors and resulting new particle formation and evolution of aerosol size distribution. Our new parameterization scheme predicts higher OA concentrations than the RACM-SOA-VBS scheme in WRF-Chem, and agrees better with measurements of size distribution evolution due to aerosol aging compared to the default RACM-SOA-VBS scheme.

1. Motivation: SOA formation mechanisms govern aerosol size distribution evolution

Quasi-equilibrium growth
Volume-determined, Raoult’s law

Diffusion-limited growth
Surface-determined, no Raoult’s law

> New laboratory results showed that SOA is formed kinetically by diffusion-limited growth (Ripinen et al., 2011; Perraud et al., 2012).
> Current chemical models usually describe SOA formation using absorptive partitioning theory, assuming instantaneous equilibrium between gas and particle phases and only consider the SOA mass.

Our idea: based on the diffusion-limited growth process, we developed a highly computationally-efficient moment-based parameterization scheme to describe aerosol size evolution.

2. Moment-based parameterization scheme development

I. Use 200 bins to describe aerosol size distribution. Integrate the time tendency of 2nd and 3rd moment.

The increase rate of 2nd and 3rd moment is determined by the diffusion-limited growth.

K: aerosol bins S: organic vapor with different volatility

\[ \frac{dM_2}{dt} = \frac{(P_N D - P_N D \exp(-\Delta S))}{RT} \]

\[ \frac{dM_3}{dt} = \frac{(P N D - P N D \exp(-\Delta S))}{RT} \]

II. Parameterize f1, f2, f3, f4 numerically

We first use detailed aerosol bins to calculate the four factors and then parameterize them as the function of \(M_0, M_2, M_3\).

Take f1 as an example:

\[ f_1 = \frac{M_2}{M_3} \exp(-\Delta S) \]

For log-normal size distribution, \(D_m, \sigma\) is calculated by \(M_0, M_2, M_3\).

III. Comparison of parameterized and bin-calculated time tendency of 2nd and 3rd moments

Our parameterization reasonably captured the size distribution difference for aerosol aging process. From June 13th to June 16th, the median diameter grows from 0.015 μm to 0.025 μm.

The difference between solid and dotted lines shows SOA contribution to aerosol size distribution. SOA formation makes aerosol size grow larger.

1. median diameter: 0.007 to 0.015 μm
2. median diameter: 0.02 to 0.025 μm

Take home message: We developed a moment-based computationally efficient parameterization to improve simulated impacts of SOA on the evolution of aerosol size distribution.

References:
1. Chen et al. (2013): A statistical–numerical aerosol parameterization scheme. ACP
2. Zhang et al. (2014): Chemical composition and mass size distribution of PM1 at an elevated site in central east China. ACP