SSH-aerosol: a state-of-the art model to simulate gas/particle partitioning

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Introduction

SSH-aerosol models aerosol formation from gaseous precursors and its evolution. It can simulate the mass of aerosols, the partitioning of semi-volatile compounds as well as the mixing-state and number concentrations of particles. It is designed to be easily implemented in 3D Eulerian models, such as air-quality models, or to be used as a box model to estimate the formation of secondary aerosols (gas and particle phases). It takes into account known phenomena involved in the formation of aerosols. The model is modular and the user can choose the complexity required (the physical and chemical processes taken into account). The model will be distributed in fall 2019. The model is based on the merge of 3 state-of-the-art models: **S**CRAM, **S**OAP and **S**SH.

Methods

SCRAM is The Size-Composition Resolved Aerosol Model. It simulates the dynamics (coagulation, condensation/evaporation and nucleation) and the mixing state of atmospheric particles. It classifies particles by both composition and size, based on a comprehensive combination of all chemical species and their mass-fraction sections.

SOAP: The Secondary Organic Aerosol Processor is a thermodynamic model that compute the partitioning of organic compounds. It takes into account several processes involved in the formation of organic aerosol (hygroscopicity, absorption into the aqueous or organic phases of particles, non-ideality and phase separation) and computes the formation of organic aerosol either with a classic equilibrium representation (the partitioning of organic compounds is instantaneous) or with a dynamic representation (where the model solves the dynamic of the condensation/evaporation limited by the viscosity of the particle)..

H^{2}O: The Hydrophilic/Hydrophobic Organics mechanism uses a molecular surrogate approach to represent the myriad of formation of semi-volatile organic compounds formed from the oxidation in the atmosphere of volatile organic compounds.

Effects of ideality and viscosity over Europe

Gas/particle partitioning over Europe was studied by implementing SSH-aerosol in the 3D air quality model Polyphemus for summer 2012. Fig 1 shows the effect of non-ideality (influencing the gas/particle partitioning) on SOA formation. Non-ideality was simulated with two thermodynamic models: UNIFAC (taking only into account interactions between organic compounds) or AIOMFAC (also taking into account the interactions with the inorganic compounds). On average over the simulation domain, similar concentrations were obtained with the two thermodynamic models but significant variations. Assuming ideality lead to a significant underestimation of SOA formation. The influence of viscosity and several other parameters on the gas/particle will also be presented.

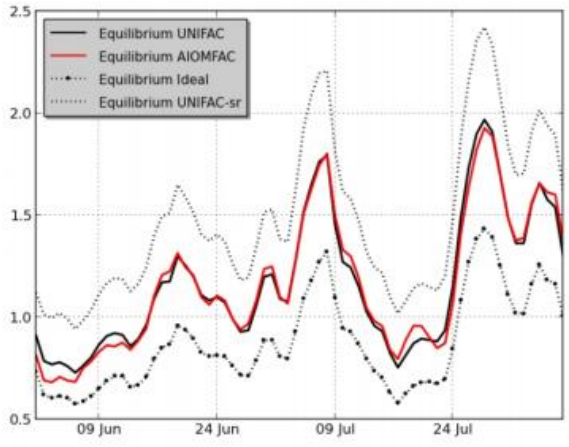

Figure 1. Effect on non-ideality on hydrophilic SOA formation.