Representation of SOA formation in air quality models: a new parameterization developed on explicit simulations

V. Lannuque[1], M. Camredon[1], F. Couvidat[2],Y.S. La[1], R. Valorso[1], A. Hodzic[3], S. Madronich[3], B. Bessagnet[2] and B. Aumont[1]

[1]LISA UMR CNRS 7583, Université Paris Est Créteil and Université Paris Diderot, Paris, France.
[2]INERIS, Verneuil-en-Halatte, France.
[3]National Center for Atmospheric Research, Boulder, Colorado, USA
Keywords: SOA formation, modelling, SOA parameterization, air quality model.
Presenting author email: victor.lannuque@lisa.u-pec.fr

Gaseous oxidation of organic compounds emitted into the atmosphere leads to the formation of thousands of oxygenated and nitrogenous organic compounds called secondary organic compounds (SOCs). A fraction of these SOCs have a volatility low enough to partition between the gas and the particulate phases, leading to the formation of secondary organic aerosols (SOAs). These SOAs represent a large fraction of fine particulate matter and contribute therefore to the impact of aerosols on air quality and climate.

In chemistry transport models (CTMs), the formation of SOA is represented with empirical parameterizations. However, comparisons with field observations show that models are not able to reproduce correctly the spatial and temporal variations of SOA mass concentrations (e.g. Solazzo *et al.*, 2012). Current SOA parameterizations are developed on the basis of smog chamber results. A direct assimilation of these results in CTM is however questionable as smog chamber experiments are usually performed during only a few hours, under conditions that differ from the atmosphere (level of oxidants and precursors, light spectrum and intensity, humidity, etc.) and with a potential artifact from wall surfaces.

The purpose of this study is to develop a SOA parameterization on the basis of deterministic simulations. A deterministic representation of processes describes the influence on SOA formation of the various environmental conditions encountered in the atmosphere. This representation is however limited by our knowledge of processes implemented in the models.

The GECKO-A model (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere) (Aumont *et al.*, 2005, Camredon *et al.*, 2007) is used to represent SOA formation explicitly. GECKO-A is a modeling tool allowing the automatic generation of explicit chemical schemes from elementary data taken from laboratory studies and structure/property relationships to estimate unknown data. GECKO-A is used here to describe the explicit formation and properties of the SOCs. The gas/particle partitioning of each SOC is described by an absorption process following Raoult's law and considering a homogeneous, ideal and inert condensed phase. The GECKO-A model has been evaluated for the purpose of SOA formation by comparison with chamber experiments (e.g. Valorso *et al.*, 2011, La *et al.*, 2016) and in situ measurements (e.g. Lee-Taylor *et al.*, 2011).

Different simulations were performed under various environmental conditions (NO_X, organic aerosol seeds, and temperature) using GECKO-A in a box-model. The simulations were used to (i) explore the distributions of the physico-chemical properties (volatility, enthalpy of vaporization, molar mass, etc.) of species produced during organic compound oxidation; and (ii) to build and optimize a parameterization for SOA formation. The gas/particle partitioning of a given SOC depends mainly on its volatility. The SOC distribution was therefore parameterized according to volatility bins, as previously done in the volatility basis set parameterization (Donahue *et al.*, 2006). The gas-phase oxidation of SOC has a large impact on the evolution of each volatility bin. The oxidation of the gaseous fraction of each bin was thus included in the parameterization. Seven bins are considered in the parameterization (called VBS-GECKO). VBS-GECKO includes SOA formation from various precursors (alkanes, alkenes, terpenes) and the impact of organic aerosol seeds, temperature and NO_X levels. The relative errors between the VBS-GECKO parameterization and explicit GECKO-A simulations do not exceed 15% on the simulated SOA mass.

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