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Development of new parameterizations for SOA production from SVOC and IVOC oxidation

Vincent Lemaire, Isabelle Coll, Marie Camredon, Bernard Aumont, and Guillaume Siour
LISA, Université Paris-Est, 94 010 Créteil ; Université Paris-Diderot, 75013 Paris ; UMR 7583 CNRS, Créteil, France
(vincent.lemaire@lisa.u-pec.fr)

Recent experimental studies have demonstrated the partially volatile pattern of primary organic aerosol (POA) that is actually associated with organic species of so-called intermediate volatility (IVOCs), and by semi-volatile (SVOCs) species. Indeed, 50% to 75% of the total emitted mass of POA may be present in the atmospheric gas phase in accordance with the thermodynamic properties of its components (Shrivastava et al., 2006). During the processing of the emission plume, this gaseous material will then undergo photochemical oxidation, enhancing the production of secondary organic aerosol (SOA) (Robinson et al., 2007; Hodzic et al., 2010; Lee-Taylor et al., 2011). Considering POA as non volatile in Chemistry Transport Models (CTMs) could thus lead to an underestimation of SOA and an overestimation of POA (Aksoyoglu et al., 2011) and bias the temporal formation of the organic aerosol (Kroll et al., 2007; Presto et al., 2012). However, very rare experimental data exist on the fate of these species and their aerosol yield, but all existing studies have shown a significant SOA production (Presto et al., 2009; Miracolo et al., 2010; Lambe et al., 2012).

Our works aims at including and testing in the CHIMERE CTM new parameterizations of SOA formation from the oxidation of IVOCs and SVOCs, arising from explicit 0D-model experiments. Our approach is based on the works of Aumont et al., (2013) who used the GECKO-A tool (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere) to generate the explicit chemistry and gas-particle partitioning of superior alkanes and their oxidation products. Using this explicit scheme, Aumont et al., (2013) indeed produced 0D simulations of the oxidation of given SVOCs and IVOCs under different initial conditions of organic aerosol mass. We first focused on the chemistry of n-hexadecane. From the 0D-experiments, we tested the influence of the number of first generation surrogate species and the number of generation taken into account in the parameterization. The stoichiometric coefficients and partitioning constants of surrogates are optimized so as to fit the 0D kinetic yield of SOA from n-hexadecane under different conditions. The obtained set of reactions is designed to be included in the CHIMERE model chemical scheme, together with that of other IVOCs and SVOCs, in order to on improve our capacity to represent organic aerosol formation in anthropogenic plumes.