Explicit modeling of SOA formation during smog chamber experiments: impact of the competition between gas/wall and gas/particle partitioning

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A main process driving the formation of secondary organic aerosols (SOAs) in the atmosphere is the condensation of low volatility compounds produced by the oxidative processes of intermediate volatility organic compounds (IVOCs). To study these mechanisms, smog chambers are widely used in the scientific community. Most of these facilities are built with Teflon material. However, several studies have reported vapor organic losses occurring onto Teflon walls in significant amounts and short timescales (e.g. Yeh and Ziemann, 2015; Zhang *et al*, 2015). This gas uptake could compete with gas-to-particle partitioning and thus is suspected to modify the amount of SOA produced and its composition as illustrated in Fig. 1.

Matsunaga and Ziemann (2010) characterized wall losses in the smog chamber at the UC-Riverside Air Pollution Research Center (APRC) and have suggested that this process may be described as analogous to the absorption of organic gaseous compounds into the aerosol phase. During this last decade, this facility was also used to study IVOC oxidative mechanisms and SOA formation processes for a large set of linear, branched and cyclic aliphatic hydrocarbons (Ziemann, 2011) with various carbon chain lengths.

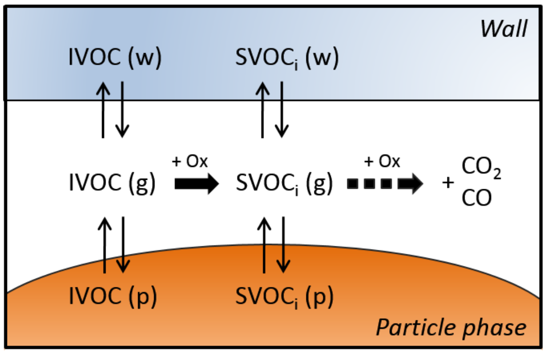

Figure 1. Schematic representation of gas/particle and gas/wall mass transfers of a semi-volatile organic compound (SVOC) produced during gaseous oxidation of IVOC (adapted from La *et al*, 2016).

The Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A) modeling tool (Aumont *et al*, 2005), describing explicitly the SOA formation and the gas-to-wall partitioning, was used here to simulated the APRC Riverside experiments in order (1) to assess the reliability of the GECKO-A model and (2) to explore the impact of vapor wall losses on SOA formation.

The model/measurement comparisons show the ability of GECKO-A to reproduce the influence of the molecular structure of the precursor on SOA formation. Without taking into account vapor wall losses, simulated results present a systematic overestimation of the measured SOA yields. Adding gas/wall partitioning into the model decreases the simulated SOA yields by as much as a factor 2 providing a better agreement with the observations. The gas/wall partitioning of organic compounds also affects the SOA chemical composition. Results clearly suggest that gas/wall partitioning is a major process influencing SOA production and composition in Teflon chambers (La *et al*, 2016).

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