MODELING THE MULTIPHASE OXIDATION OF ORGANIC CARBON: AN EXPLICIT APPROACH

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Context
Secondary organic species are usually multifunctional species with high water solubility and/or low vapor pressure (Fig. 1). They can therefore partition between the gas and condensed phases. These secondary species mostly: 

- physical and chemical properties of aerosols by secondary organic aerosol formation.
- cloud chemistry (e.g. acid formation) and microphysics (e.g. surface tension effect, properties of aerosols acting as CCN).

Fig. 1: Evolution of carbonaceous species simulated during n-heptane oxidation. (a) distribution of organic carbon. (b) distribution of secondary C7 organics as a function of the number of functional groups borne by the molecules. (c) representative C7 species of organics bearing 2 and 4 functional groups. [1]

Objective
An explicit approach for organic multiphase oxidation modeling imply the development of an expert system that:

- describes partitioning of the organics between the various phases (i.e. describe mass transfer and provide the related parameters: Henry's law constants, vapor pressures, activity coefficients, ... (Fig. 3)).

Example: vapor pressure estimates
Vapor pressure is a fundamental property controlling gas-particle partitioning and therefore a critical parameter for modeling the formation of secondary organic aerosols (SOA).

Various estimation methods were recently assessed for the purpose of SOA modeling [3]. It was found that the Myrdal and Yalkowsky method [3] provides vapor pressure estimates with a good accuracy (Fig. 5).

Explicit gas/particle partitioning modeling

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The model is based on the gas-phase scheme described in [1], in which gas-particle equilibriums are applied at each time step, assuming (i) an absorption process and (ii) that the aerosol phase behaves as an ideal phase. Vapor pressures are estimated with the Myrdal and Yalkowsky method [3].

Conclusion

The development of explicit modeling is a necessary step to test our current understanding of the evolution and impact of organic carbon during its atmospheric oxidation.

Data processing tools are required to (i) assimilate the various experimental data provided by laboratory studies, (ii) codify the various estimation methods and (iii) generate consistent and comprehensive oxidation schemes on a systematic basis.

The expert system for organic multiphase oxidation self-generates explicit gas-phase oxidation schemes and describe gas-aerosol mass transfer. Although preliminary, the results are very promising and show the potentialities of a self-generating approach for organic carbon modeling.

References: