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The Secondary Organic Aerosol Processor (SOAP v1.0) model: a unified model with different ranges of complexity based on the molecular surrogate approach

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To parameterize the morphology factors of a particle with a solid core, the diffusion of organic compounds inside an ideal particle of constant diameter is treated explicitly as described in the following section. The evolution of the concentration of organics as a function of time is explicitly computed for different solid volume fraction f_s. For each f_s, morphology factors are fitted to reproduce the results of the explicit evolution of organics with the simplified approach presented in this paper. The polynomial parameters were then fitted to represent the evolution of the morphology factors with f_s.

1 Discretization of the diffusion of organics inside a particle with a solid core

The flux F (in molecules/s) of molecules crossing a surface S by diffusion is:

$$F = S D_{org} \nabla C \tag{1}$$

By discretizing this equation for a sphere (where concentrations only depend on the radius r to the center of the particle), the flux of molecules crossing the interface between a layer i of mean radius R_i and a layer j of mean radius R_j (with j=i+1 or j=i-1) is:

$$F_{i,j} = 4\pi r_{i,j}^2 D_{org} \frac{C_j - C_i}{R_j - R_i} \tag{2}$$

where $r_{i,j}$ is the radius to the center of the particle of the interface between the layers i and j.

To solve the diffusion of organic compounds into a particle with a solid core, the organic phase is descretized into N_{layer} (equal to 100) layers from r = R_s the radius of the solid core to r=R_p the radius of the particle. By definition of the volume fraction of the solid core f_s:

$$R_s = R_p f_s^{1/3} \tag{3}$$

The radius $r_{i,i+1}$ is computed by:

$$r_{i,i+1} = r_{i-1,i} + (R_p - R_s)/N_{layer} \tag{4}$$

with i varying from 1 (for the layer at the interface with the solid core) to N_{layer}-1 (N_{layer} being the index for the layer at the interface with the gas phase) and with $r_{0,1}$ being the radius of the solid core R_s.

The radius of the layer R_i is computed by:

$$R_i = 0.5 \left(r_{(i-1,i} + r_{i,i+1} \right) \tag{5}$$

The evolution of concentrations inside layers is described by:

$$C_i(t + \Delta t) = C_i(t) + \frac{F_{i,i+1} + F_{i,i-1}}{V_{layer}} \Delta t \tag{6}$$

with V_{layer} the volume of the layer.

$$V_{layer} = \frac{4}{3}\pi \left(r^3_{i,i+1} - r^3_{i-1,i}\right) \tag{7}$$