A molecular dynamics study on the morphology of ultrafine multicomponent organic aerosol

Katerina S. Karadima [1,2#*], **Vlasis G. Mavrantzas** [1,2,3] and **Spyros N. Pandis** [1,2,4]

[1]Department of Chemical Engineering, University of Patras, Patras, 26504, Greece

[2]Institute of Chemical Engineering Sciences, FORTH/ICE-HT, Patras, 26504, Greece

[3]Department of Mechanical and Process Engineering, ETH Zürich, Zurich, 8092, Switzerland

[4]Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, 15213, USA

Presenting author: Katerina S. Karadima, email: kkaradima@chemeng.upatras.gr
* Corresponding author: Katerina S. Karadima, email: kkaradima@chemeng.upatras.gr

ABSTRACT

Organics are abundant and quite omnipresent in atmospheric particulate matter, which plays an important role in air quality, human health, and earth's climate. Evaporation, condensation, and heterogeneous chemical reactions are the most important processes that atmospheric aerosol undergoes during its lifetime. These processes are affected by many factors, which include also phase state and morphology. Aerosol phase state and morphology have an impact on water uptake, bulk and gas/particle diffusion rates, heterogeneous reactions rates, cloud droplet formation, aerosol lifetime and optical properties. The study of the morphology of ultrafine particles is quite difficult to be determined with a typical experimental setup. The method of molecular dynamics simulation can, however, provide valuable insights into the morphology of particles in that scale and information about their physicochemical properties.

The morphology of multicomponent organic/inorganic aerosols under atmospherically relevant conditions is explored in this work. A variety of organic compounds is used (*cis*-pinionic acid/CPA, 3-methylbutane-1,2,3-tricarboxylic acid/MBTCA, linear alkanes, and mixtures of them) together with typical inorganic compounds (sulfate, ammonium, and water), and, nitrogen and oxygen for the gas phase. The particles are allowed to form spontaneously in the course of the molecular dynamics simulation, which is performed in the isothermal–isobaric (N*p*T) statistical ensemble. The particle microstructure is studied after its equilibration and relaxation. The effect of relative humidity, organic mass content and type of organic compound in particle morphology is investigated for a wide range of relative humidity values and organic mass fractions.

Phase separation is observed for the majority of the simulated nanoparticles either between organics and inorganics or between hydrophilic and hydrophobic components. For most of the cases the ions separate from the organics. The organic–rich phase is located at particle surface and depending on the relative humidity and organic mass fraction organic islands up to core–shell structures can be observed.[1] The surface enrichment in organics is enhanced as the humidity increases. The presence of organics in the interior of the nanoparticle increases with their mass fraction, but this increase is also humidity dependent. Separation is also predicted between primary and secondary organics or even between secondary oxidation products (CPA and MBTCA) under certain conditions, where the less oxidized compound resides at the surface of the particle.[1]

REFERENCES

[1] Karadima KS, Mavrantzas VG and Pandis SN. 2019. *Atmos. Chem. Phys.*, **19**:5571 – 5587.