CFD simulations to enhance the performance of an axial mobility classifier for ionic molecular clusters

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New particle formation is one of the most active research areas in atmospheric sciences. The development of new instrumentation like (CI-) APi-TOF mass spectrometry (MS) (Junninen et al., 2010, Jokinen et al., 2012) considerably increased the understanding of the mechanisms of new particle formation with respect to the participating trace gases (Almeida et al., 2013, Schobesberger et al., 2013, Kirkby et al., 2016). The instrumentation used so far such as the (CI-) APi-TOF MS might however not detect the exact composition of nucleated clusters as loosely bound ligands are likely to evaporate from these clusters during the charging or ion guiding process inside the instrument.

This lack of knowledge motivated the development of a prototype MS with an axial mobility classification (AMC) inlet. We optimized the transition region into the high vacuum part of the MS providing a soft and low fragmenting transition, which makes the so called "nanoTOF" especially suited to study fragmentation and evaporation processes of ionic molecular clusters.

The operating principle of the AMC follows the same concept as presented recently by Bezantakos et al. (2015) and Tammet (2015). By applying a defined electric field opposite to the sample flow, only ions beyond a specific electrical mobility are able to pass the electric field and to further enter the MS.

For the newly developed nanoTOF inlet, two parameters are critical for detailed studies on the composition of nucleating atmospheric clusters: first, the overall transmission efficiency from ambient (atmospheric) pressure to the detector of the MS at high vacuum; second, the resolution power of the electrical mobility classification.

To this end, besides laboratory experiments, computational fluid dynamic (CFD) simulations of ion trajectories in the AMC inlet were performed using the open-source CFD software *OpenFOAM* (www.openfoam.com). The motion of ions was simulated for different setups changing the flow rate, electric field strength or inlet geometry. As an example, Fig. 1 shows simulated flow profiles of ions of three different mobility diameters. Larger ions (red) are slowed down less by the electric field than small ions with a higher electrical mobility (white and blue). While the strength of the electric field is efficiently used to select different electrical mobilities, the simulations showed that the shape of the electric field and the flow rate determine the transmission through the core sampling inlet and the resolution power.

The CFD simulations represent an important tool for the study of the transmission properties of ions of different electrical mobility (or mobility diameters respectively). They will therefore help to further optimize the transmission and resolution power of the AMC inlet of the nanoTOF, allowing a proper classification of nucleating atmospheric clusters.

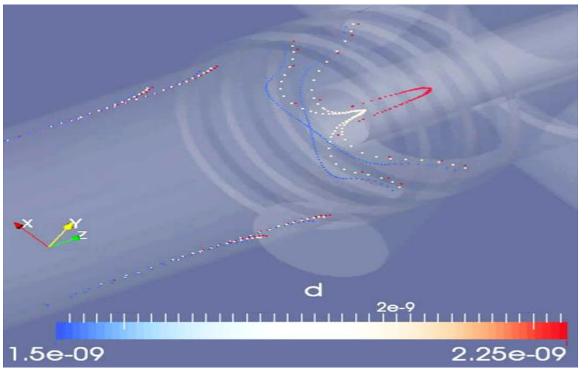

Fig. 1: Simulation of an ion flow through the core sampling inlet for ions of three different mobility diameters, *d*: 1.5 nm (blue), 2.0 nm (white) and 2.25 nm (red).

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