Session of Focus Materialchemie – Thursday, **24.10.2024** 11:00 @ Seminarraum Lehar 02 (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46)

Inverse aerosol dynamics: from instrument data inversion to estimation of microphysical process rates

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A direct model of an aerosol instrument is such that if the aerosol size and chemical composition distribution as well as the instrument details are known, the model outputs the instrument signal, i.e. what is typically called raw data. In case of a typical device which is based on particle charging and measurement of electrical mobility, such as in the case of a differential mobility particle spectrometer (DMPS), the raw data consists of counts vs voltage. Conversely, an inverse model of a single DMPS measurement tries to estimate the aerosol size distribution based on the raw data. This inverse problem is typically ill-posed, which means that there can be an infinite number of different size distributions that result in a similar instrument signal [1]. One additional source of difficulty is uncertainties in the instrument – in the case of a DMPS especially related to the aerosol charging process [2]. Our aim is, with given raw data and taking into account the uncertainties, to estimate the most probable size distribution as well as its uncertainties using Bayesian methods [3, 4].

In modeling aerosol dynamics, a direct model predicts the evolution of the aerosol size distribution when the conditions are known (from which coagulation, condensation, nucleation and deposition rates can be calculated) by numerically solving the aerosol general dynamic equation (GDE). In our inverse modeling work, our aims are twofold: 1. to estimate an earlier size distribution from measurements after dynamics has taken place [5], and 2. to estimate the microphysical process rates from a time series of size distribution measurements [6]. Again, our methods of choice are Bayesian: MCMC, Extended Kalman filter and Extended Kalman Smoother [3]. These methods have not been used widely in aerosol dynamics, but based on our initial work are very promising especially when uncertainty estimation is an important goal. One additional novelty of our work is coupling finite element method based solution of the GDE to the Bayesian inverse framework [7].

As example calculations we have studied synthetic data (for which the ‘answers’ are known), aerosol chamber experiments and dynamics of automobile tailpipe emissions.

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