Integrated ion trajectory simulations in OpenFOAM, an open source framework for complex numerical simulations

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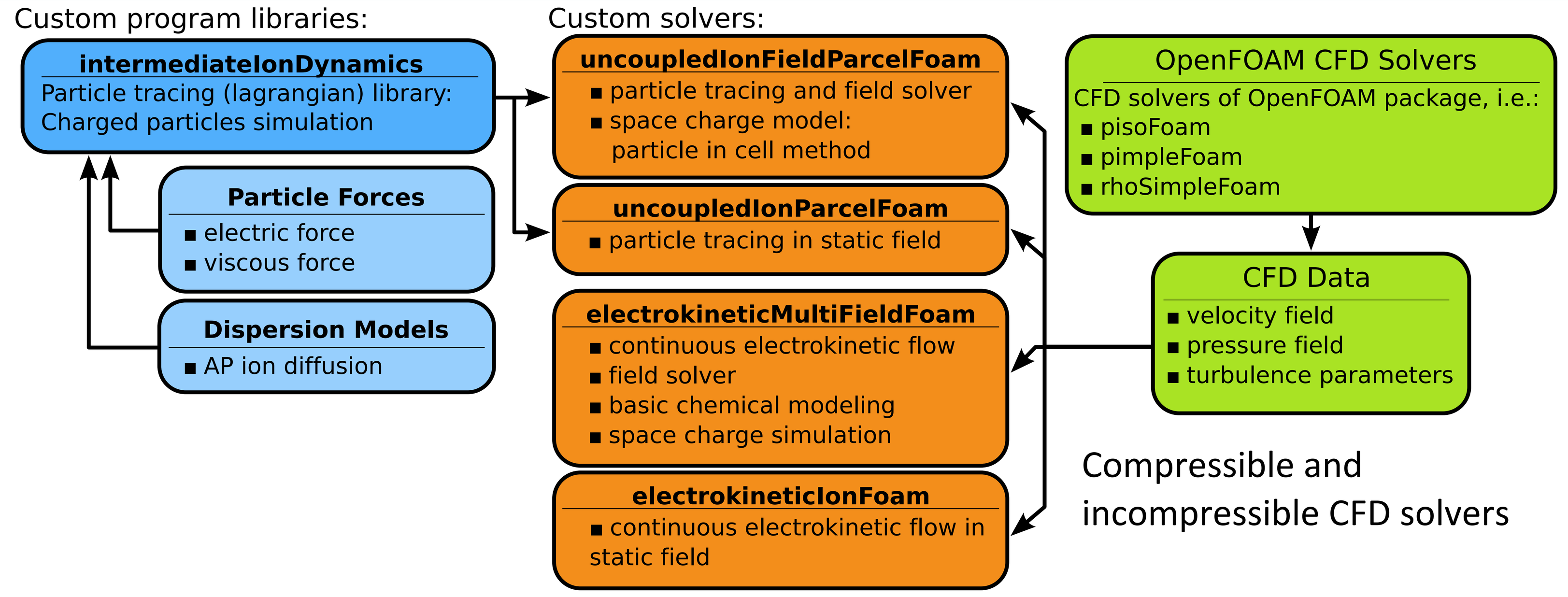
Introduction

In the past years, the numerical simulation of ion trajectories at elevated background gas pressures based on computational fluid dynamics (CFD) has become readily feasible with commercial tools (Comsol, CFX, Simion) [1,2,3]. Despite the possibilities provided by these programs, they have certain disadvantages, e.g. lack of multicore support, lack of advanced flow models and inaccessibility of the core source code.

In contrast, the open source simulation framework **OpenFOAM** provides an accessible, integrated base for coupled multiphysical simulations as for example ion trajectory calculations.

We present a set of custom OpenFOAM solvers for the calculation of the motion of charged particles at atmospheric pressure. The results of exemplary simulation problems are compared with results obtained using established commerical tools.

Custom Simulation Codes



Methods

Software Tools:

Solvers:
- OpenFOAM v2.2.2
- Comsol Multiphysics v4.4
- SIMION 8.1.1.32 with SDS model

OpenFOAM mesh generation:
- Salome 6.3.0
- blockMesh

OpenFOAM result visualization: Paraview 4.1.0

Additional result analysis generation: NumPy and Matplotlib Python libraries

Hardware:

advanced consumer class computer:
- Dell Precision T7400 Workstation (Xeon E5530 CPU)
- Apple iMac (Core i5 CPU)

OpenFOAM: Future Options

The presented demonstration models prove that OpenFOAM is applicable to simulation problems in mass spectrometry and ion source development.

The open structure of OpenFOAM allows the rapid development of new custom solvers and combination with existing software.

Planned development options for the OpenFOAM package are:

Low pressure transsonic fluid dynamics

The presented models are applicable for high pressure conditions. OpenFOAM allows also the simulation of transsonic gas flows under low pressure conditions (e.g. by DSMC via dsmcFoam)[4,5]. To combine these solvers with ion trajectory simulations, low pressure gas collision models have to be developed.

Chemical modeling in particle tracing simulations

Adaption of the recently published Reaction Simulation (RS) method [5] for particle based simulations in OpenFOAM

Charged droplets / droplet breakup

It is envisioned that the simulation of the dynamics of charged droplets gains deeper insight into the overall dynamics of ESI processes

Simulation Results: Exemplary Simulation Cases

Drift Channel including Ion Chemistry

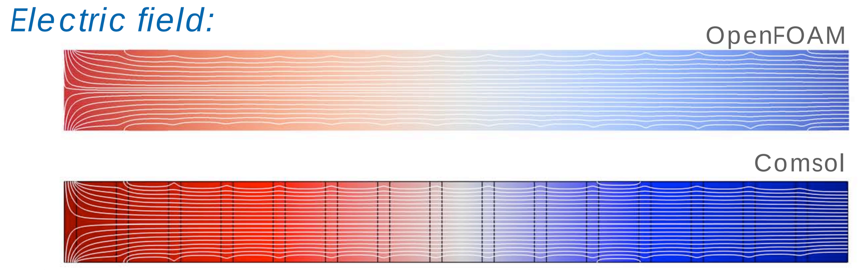
The motion of two ionic species ("A", "B") in a drift channel (200x20 mm) with stacked ring electrodes was simulated with Comsol and OpenFOAM. The ionic species are simulated as continuous concentration field (electrokinetic flow). The gas flow (1 m/s inflow velocity) as well as the electric field (linear drift field, 4kV on first electrode) were also simulated using both solvers.

Ion Chemistry

To demonstrate the basic ability to simulate reacting ion flows, the ionic species was assumed to be reactive:

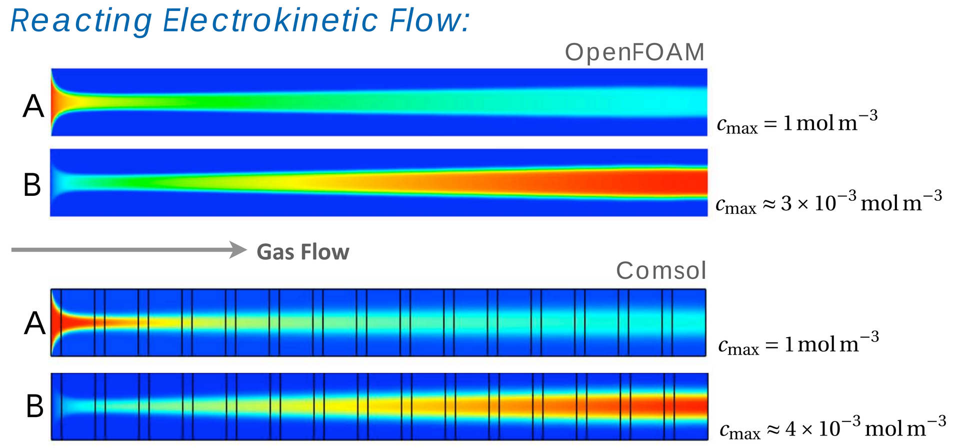
$$A \xrightarrow{k_a} B \qquad B \xrightarrow{k_b} A$$
$$k_a = 0.5\,\mathrm{s}^{-1} \qquad k_b = 0.001\,\mathrm{s}^{-1}$$

Electric field:



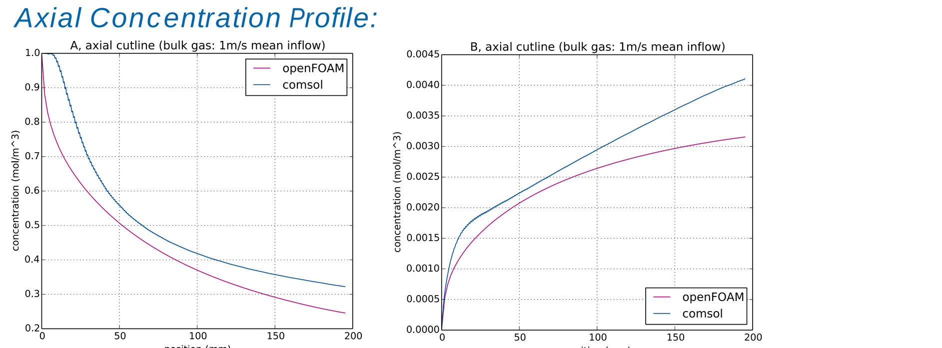
above: Simulation of the electric potential and field lines, the solutions are essentially identical

Reacting Electrokinetic Flow:



above: Simulation of the spatial concentration distribution in the drift channel.

Axial Concentration Profile:



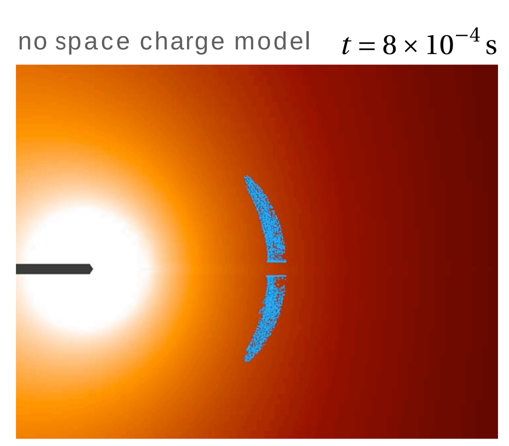
above: The axial concentration profiles reveal a noticeable difference between the solutions

Space Charge: Particle in cell model

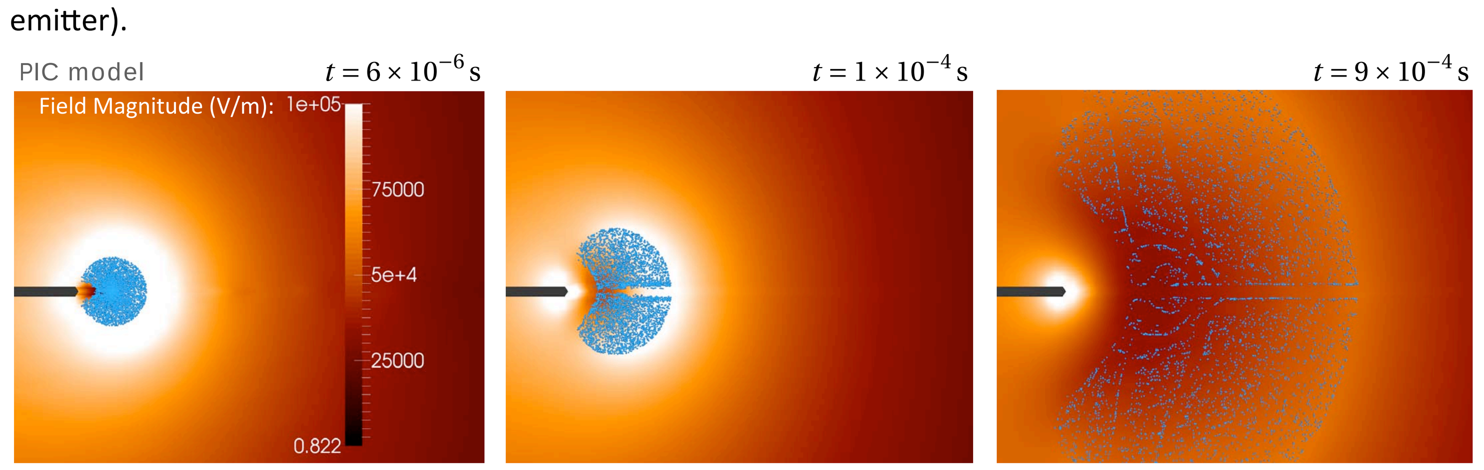
One option to model space charge in a particle based simulation is projection of the charged particle density back onto the discretization mesh. In the subsequent time step the electric field distribution is calculated considering the charge density induced by the particles. This is known as the **Particle in Cell** (PIC) method.

The particle tracing library of OpenFOAM provides the required particle density which allows the rapid implementation of a PIC solver for ion motion at AP conditions.

The proof-of-concept simulation shows the emission of ions from a needle shaped field emitter with 500 µm diameter (e.g. an ESI emitter).



left: A particle tracing simulation without the PIC space charge model clearly differs from the result with space charge modeling (*below left*)



left: With activated PIC model, the effect of the charged particles on the field distribution (field shielding) is clearly visible.

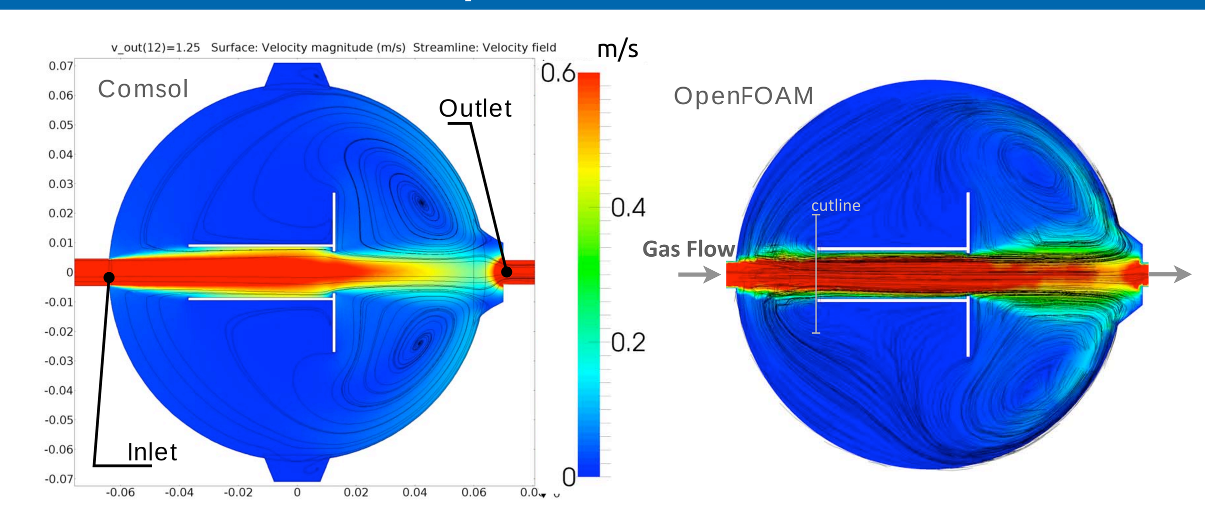
Also, the effects of the changed charge distribution on the particle cloud (coulomb repulsion and field shielding) is visible.

Ion Deflection in an Atmospheric Pressure Measurement Chamber

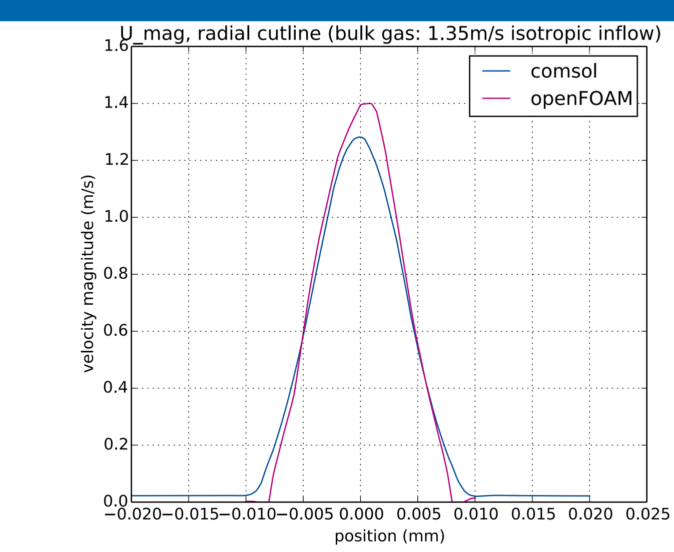
Bulk Gas Flow:

A measurement setup was simulated which has been used in the past for the experimental verification of numerical ion transport models [ref]. It consists of a cylindrical measurement chamber at atmospheric pressure conditions. A bulk gas flow (1.25 m/s mean inflow velocity) transports ions from an ion source through this chamber.

We have simulated the gas flow with Comsol and OpenFOAM. The results have been used for ion transport simulations (below).



above: Bulk gas flow (velocity magnitude and stream lines) in the measurement chamber. Despite some noticeable differences, the results are in good overall agreement.



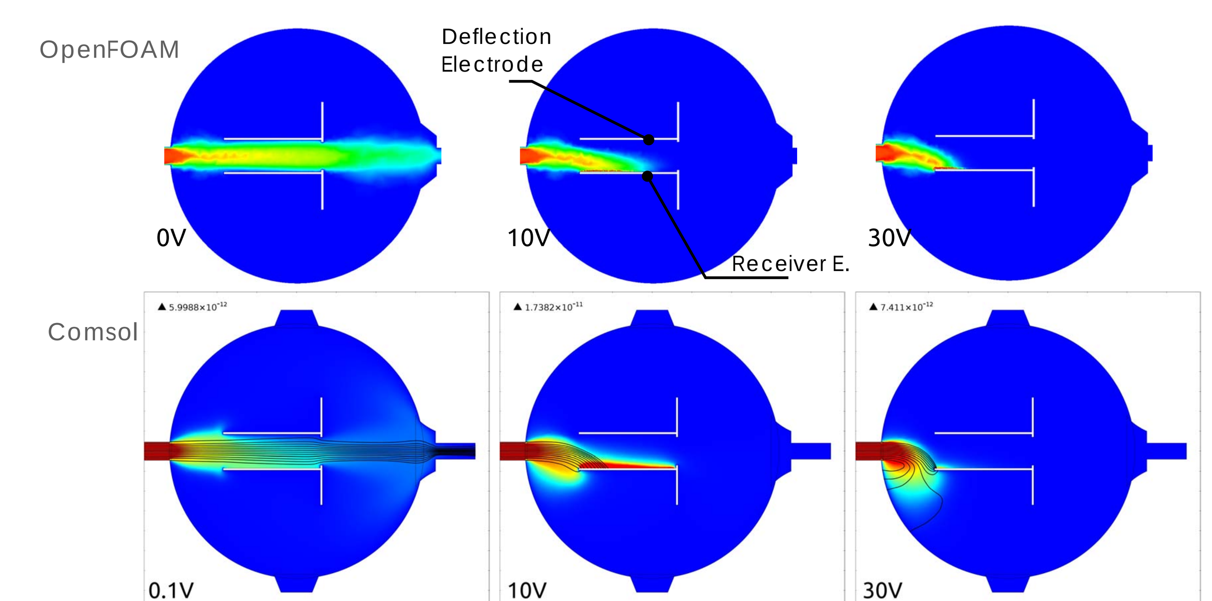
above: Velocity magnitude on a cutline trough the main gas stream (as marked on the left).

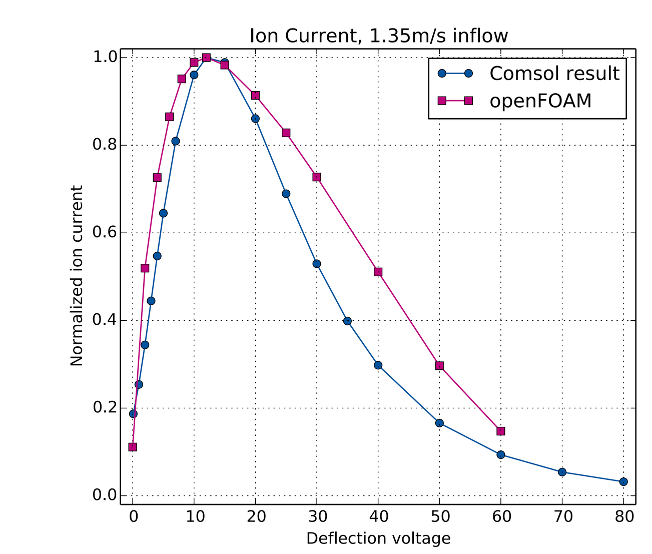
Electrokinetic Flow:

Ions generated in an upstream ion source are transported into the measurement chamber by the bulk gas flow. In the chamber, the ions are deflected by an electric potential on a deflection electrode. The ion current on a parallel receiver electrode was measured in previous experiments to verify the Comsol and SIMION model presented here (see [2] for details).

The electrokinetic flow of the ions was simulated with OpenFOAM and the results are compared with Comsol calculation results.

Both solvers give similar results for the deflection voltage dependence.



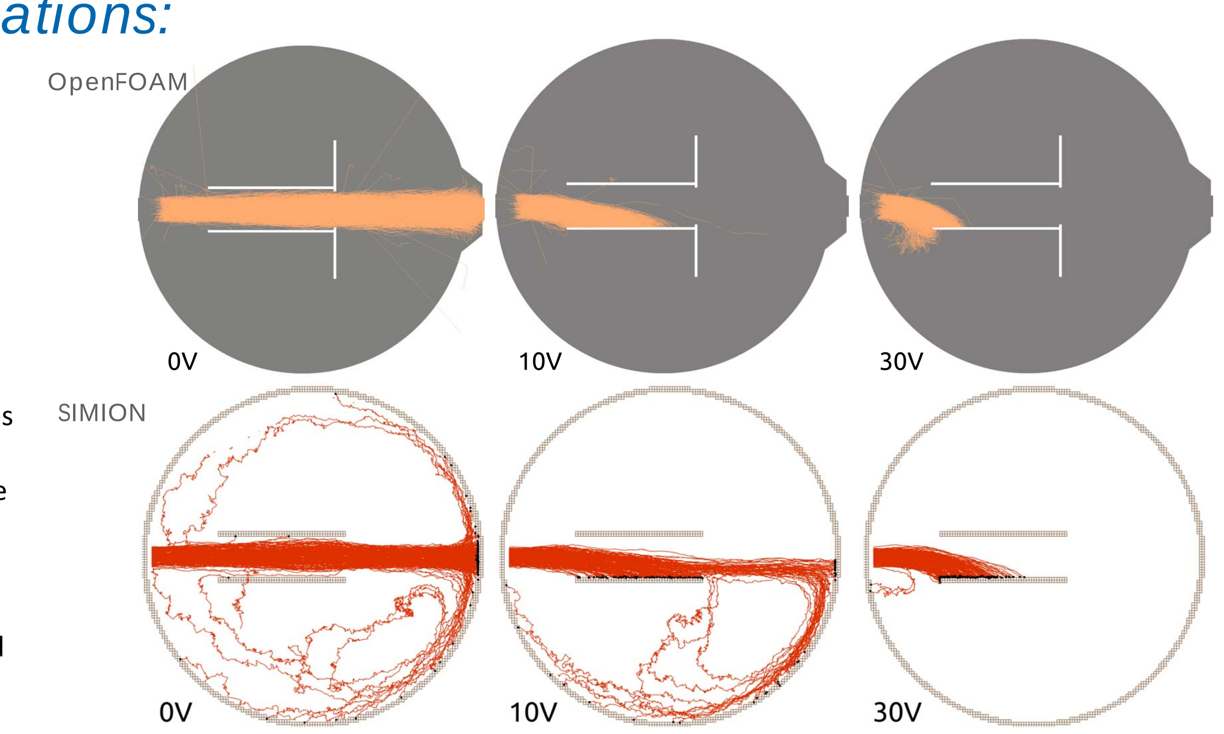


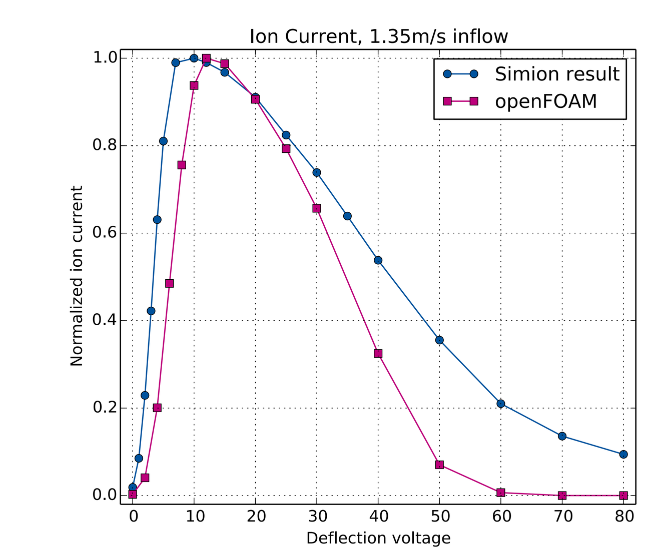
Particle Tracing Simulations:

The transport of ions in the measurement chamber was also simulated with a particle tracing model. The resulting particle trajectories are compared with results obtained with SIMION with the Statistical Diffusion Simulation (SDS) collision model.

The particle tracing calculations performed with OpenFOAM and SIMION on the deflection voltage dependence show noticeable differences. The simulated particles exhibit a higher electrical mobility in the OpenFOAM calculations. In comparison to the electrokinetic flow simulation (*above*), the differences between the models are larger in the particle tracing calculations.

Interestingly, the difference in the normalized ion current on the receiver electrode (*far right*) is relatively minor.





above: The simulated ion current on the receiver electrode shows good qualitative agreement between SIMION and OpenFOAM or Comsol and OpenFOAM, despite the visible differences in the particle trajectories and in the electrokinetic flow pattern (*left, left above*).

Conclusions

- A solver for electrokinetic flow and a particle tracing solver for the simulation of ion trajectories have been developed based on the OpenFOAM framework
- The simulation results obtained with the new solvers are in good qualitative agreement with the results from commercial solvers (SIMION, Comsol)
- A particle in cell solver was developed which is currently not commercially available
- The PIC solver combines space charge and particle based ion transport models which allows simulations of ion motion in high space charge regions
- Basic chemical reaction modeling is demonstrated for the electrokinetic flow simulation
- The overall results show that OpenFOAM is a highly valuable tool for ion dynamics simulations at atmospheric pressure
- Despite the good overall agreement, noticeable differences between the solutions are apparent
- Future research will investigate the causes for these differences
- The freely accessible structure of OpenFOAM provides a wide range of future development options which is particularly valuable for experimental numerical models in fundamental research

Literature

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