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

Walter Wißdorf; Thorsten Benter

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 freedom support, bolt of validated flow models and insufficiency of the ion source code.

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

We present a set of OpenFOAM solvers for the calculation of the motion of charged particle at atmospheric pressure. The results of exemplary simulation studies are compared with results obtained using established commercial tools.

Custom Simulation Codes

- Particle Pathway Analysis
- Multiphase Simulations
- Collision Models
- Reaction Models
- Space Charge Models
- Particle Trajectory Analysis
- Simulated Results
- Conclusions

Simulation Results: Exemplary Simulation Cases

Drift Channel including Ion Chemistry

- Simulation results obtained using established commercial tools (Comsol, CFX, Simion).

- These programs have certain disadvantages, e.g. lack of freedom support, bolt of validated flow models and insufficiency of the ion source code.

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

- We present a set of OpenFOAM solvers for the calculation of the motion of charged particle at atmospheric pressure. The results of exemplary simulation studies are compared with results obtained using established commercial tools.

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 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 post-oc simulation shows the emission of ions from a needle shaped field emitter with 500 μm diameter. (as an ESI emitter).

- PIC, model.

- With PIC model, the effects of the charged particles on the electric field distribution are clearly visible.

- Also, for the effects of charged particle cloud simulations, the software tools OpenFOAM and Comsol are used.

Methods

- Software Tools:
  - OpenFOAM v.2.3
  - COMSOL Multiphysics v.4.4
  - SIMION 8.1.2.1.32 with SMD model

- OpenFOAM mesh generator:
  - Smedley 3.10
  - BruchWeb

- OpenFOAM result visualization:
  - ParaView 4.0

- Additional result analysis generation:
  - NumPy and Matplotlib Python libraries.

OpenFOAM: Future Options

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

- Planned development options for the OpenFOAM package are:
  - Chemical modeling in particle tracing simulation
    - Adaptation of the previously published Reaction Simulation (RS) method [4] for particle based chemical reactions
    - Charged droplet/droplet break up
      - It is envisioned that the simulation of the different charged droplet gas dynamics insight into the overall dynamics of the process.

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 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.

- Financial support by GenSax UF (Hanns, Germany).

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