Integrated Ion Dynamics Simulations in OpenFOAM:
Flow, Transport, Chemical Reactions, and Space-Charge

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Introduction

Chemical reactions play a crucial role in the understanding of AP-IMS and associated methods, e.g. ion mobility spectrometry (DIMS). Thus, the numerical simulation of the ion dynamics in analytical instruments must incorporate a model of the chemical dynamics of the ions (2-5). We presented an open-source framework based on OpenFOAM for the simulation of ion trajectories under various conditions. The framework was extended with modules for the statistical simulation of chemical kinetics (DIMS), the simulation of the effective ion-surface temperature, and low pressure collision model (hard sphere collisions). This approach paves the way for the simulation of highly dynamic processes under viscous and rarefied pressure conditions.

Methods

Software Tools / Frameworks:
- OpenFOAM 2.3
- RadFlow 3.0
- OpenDMD

Calculation Matlab Environment:
- Lattice Boltzmann Model

Additional Analysis Libraries:
- Numpy, Scipy, and a Python interpreter

CFD Codes:
- IJSJ Ballistic Code
- SIAM, MRT

Ion Trajectory and Kinetics Simulation:
- Set of custom-built libraries and solvers ("Turnkey"")

Hardware:
- Dell Precision T7600 Workstation (Quad X5670, 4.0 GHz)
- Apple Mac (G4)
- Custom-built cluster (OpenFOAM 6282)

Reacting Ions: Reactant Ion Peak in Ion Mobility Spectrometry

The signal of proton bound water clusters in high pressure Ion Mobility Spectrometry (IMS) is the so-called Reactant Ion Peak (RIP). It is an ideal benchmark problem for the simulation of the chemical dynamics of gas phase ions under viscous conditions.

Lattice Boltzmann Model Simulation of Gas Flow in the IMS device
- Gas Velocity (m/s)
- Separation Plate Voltage

Reactive Collision Models
- DSMC CFD
- Ion Tracking Simulation
- Particle in Cell
- Lattice Boltzmann Method

Chemical Kinetics: Equilibrium of the System

The equilibrium of the water cluster system in an AP-IMS (gas-in vacuo) is simulated using the OpenFOAM DSMC simulation. The results of the simulation of the water cluster system with Smolin/RS methods and the OpenFOAM based simulation agree well. The stable right step deviation potentially contributes to the deviation of the simulated drift time shown on the left.

Conclusions

- A simulation framework ("IonFoam") based on OpenFOAM was developed.
- The framework can be coupled with a wide range of CFD methods. Particularly, methods suitable for the simulation of rarefied gas flows (Lattice Boltzmann methods and DSMC) can be combined with IonFoam.
- The framework incorporates models for chemical kinetics, the effective reaction temperature of reactive gas phase ions, and space charge.
- The calculations can be parallelized and run on cluster computer systems. Millions of particles can be simulated in a parallel calculation.
- Benchmark simulations of the chemical dynamics and drift time of the proton bound water cluster RIP in an AP-IMS reveal that the simulation of the chemical kinetics in ionFoam is valid with respect to Smolin/RS calculations as well as experimental results.
- The trajectories and reactions of proton bound water clusters in an a气质 flow through a double skimmer setup were successfully simulated.
- The chemical dynamics and separation of cluster ions in an differential mobility separation device were simulated.
- The modular design of OpenFOAM and ionFoam allows for integration of more complex collision and reaction models which e.g. consider the internal energies and degrees of freedom of the reacting particles.

Literature


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