Integrated Simulation of Rarefied Gas Dynamics and Ion Transport with a DSMC Method

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Introduction

Direct Simulation Monte Carlo (DSMC) is a well-established method to investigate the dynamics in low density gases with a particle based numerical approach. For the simulation of neutral gas flows, SPARTA (**S**tochastic **PA**rallel **R**arefied-gas **T**ime-accurate **A**nalyzer [1]), is a popular open-source DSMC code.

SPARTA handles elementary chemical reactions and arbitrary surface geometries in the simulation domain. However, albeit charged particles (charged droplets, molecular ions) are implemented in SPARTA, their interaction with external electric fields is currently not.

To widen the applicability of the code, we investigate a new module in SPARTA, which allows the simultaneous determination of the electric field force and the interaction between charged and neutral particles by the soft-sphere collision model.

To evaluate the simulations, ion mobilities are calculated and compared with literature data.

Methods

Simulations

- Modified SPARTA open source DSMC Code (based on version from jan20) [1]

Data Analysis

- Python 3 with numpy, pandas, matplotlib, scipy, vtk [2] [3]
- Paraview 5.7.0 and corresponding pvpython [4]

Machines

- Workstation Computer (Dell Precision T5700) Intel Xeon E5530, 24 GiB RAM, Ubuntu 18.04 LTS
- Compute Server, 4 AMD Opteron 6282S, 488 GiB RAM, openSUSE Leap 42.3

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Ion Mobility

Benchmark Setup

Fig 1: Generic high kinetic energy IMS; applied electric field is parallel to the main axis of the drift tube

The geometry of a high kinetic energy IMS drift tube is used as benchmark model. The two dimensional simulation consists of a IMS with a side ratio of 3:16. The pressure of the background gas is 20 mbar and reduced field strengths from 20 up to 600 Td are applied. The electric field orientation is parallel to the x axis of the simulation domain. The particles are generated in the blue area at the left. Approximately 100 charged particles are introduced in each simulation. For collisions between the charged and neutral particles the variable soft sphere collision model is used [5].

Ion Mobility

$$K = \frac{v_d}{E} \qquad \text{(Eq. 1)}$$

$$K_0 = K\frac{N}{N_0} \qquad \text{(Eq. 2)}$$

After a acceleration period, the charged particles reach a steady state drift velocity v_d. To compare the simulation results with literature data, the electrical ion mobility **K** (cf. **Eq. 1**) is calculated from the drift velocity and the electric field force E. To compare different ion mobility experiments, a normalized reduced ion mobility K_0 is calculated by correcting the ion mobility with the background gas density (N) (cf. **Eq. 2**) [6].

The differences between the calculated values of K_0 and the literature data is shown in **Fig. 2**. The blue area represents simulated data and the green area literature data [7]. The dashed/solid lines differ between the ion and background species. The difference decreases with the increasing reduced field strength. The simulated values are a factor of 3.2 up to 5.2 higher.

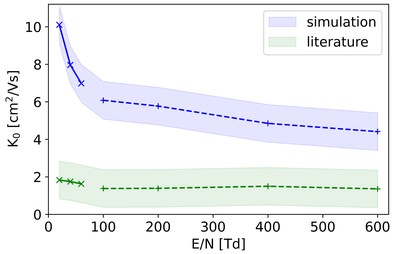

Fig 2: Simulated K_0 for N_2^+ in O_2 (solid line) and O_2^+ in CO_2 (dashed line) in comparison with literature data [7]

Observed Difficulties

Two major challenges are encountered when calculating the ion mobility via SPARTA simulations. On the one hand we have address the overestimated high ion mobilities and on the other hand unstable boundary conditions within the DSMC simulation occur.

Number of Collisions

Exclusively too high reduced ion mobilities are calculated. The ions undergo insufficient collisions to reduce their drift velocities. Therefore, too high ion mobilities are determined. Additionally, the higher the reduced field strengths are the higher is the drift velocity becomes and the smaller is the error on calculated reduced mobilities (cf . **Fig 2**).

By increasing the diameter of the charged particles in the variable soft sphere collision model, the number of collisions increases correspondingly. In **Fig. 3** the ion diameter and the corresponding reduced ion mobility is shown. By doubling the diameter twice the ion mobility falls even below the literature value (marked in green) of K_0. This shows that the overestimation of the drift velocity with accompanying underestimation of collisions with the background gas is the main cause of the discrepancies observed between calculation and experiment.

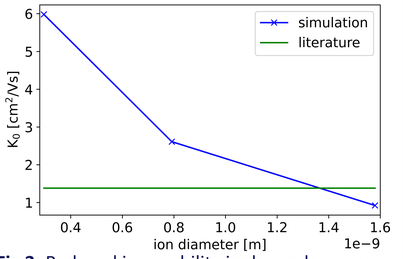

Fig 3: Reduced ion mobility in dependence on the ion diameter

Boundary Conditions

Additionally, difficulties with the boundary conditions are observed. As shown in **Fig 4** the background gas density decreases with the progress of the simulation. In some regions at the end of the simulation domain the density is decreased by a factor of two. This causes problems when the charged particles enter these lower pressure regions, because fewer collisions with the background take place; resulting in higher drift velocities.

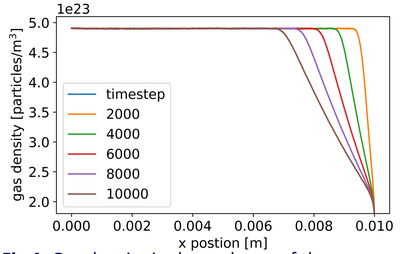

Fig 4: Gas density in dependence of the x position of the simulation box for different timesteps

Conclusion / Outlook

Conclusion

- In principal the newly introduced electric field extension for SPARTA works
- Charged particles accelerate and reach a steady state drift velocity as expected
- The calculated ion mobilities are on the correct order of magnitude but still substantially too high
- By increasing the diameter of the charged particles and the number of collisions, much better agreement between calculated and experimental ion mobilities is achieved
- Nevertheless, a reliable determination of ion mobility is yet not feasible with SPARTA simulations

Outlook

- Stabilize boundary conditions to get more robust simulation results
- Figure out if the underestimation of collisions in the SPARTA DSMC code is fixable
- Try to calculate ion mobilities with other simulation codes (e.g. custom ipaMS simulation code IDSimF)

Literature

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