Comparison and Validation of Atmospheric Pressure Ion Migration Models - Finite Element Methods vs. Discrete Particle Tracing

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In addition to the electric forces, the motion of ions under atmospheric pressure conditions is governed by the high collision frequency between the charged particles and the bulk gas. This interaction leads to particular effects, which do not occur under reduced pressure conditions:

- Viscous drag / viscous transport of ions by the motion of the neutral gas
- Molecular diffusion of ions

Thus a numerical model of the motion of charged particles at atmospheric pressure has to incorporate:

- The dynamical model of the bulk gas (fluid flow, turbulence, temperature, pressure, viscosity)
- A model of the interactions between bulk gas and ions

There are at least two distinct modeling approaches for this task:

- Formulation of a continuous transport / diffusion equation (partial differential equation - PDE) and numerical solution with the finite element method (FEM)
- Numerical simulation of discrete charged particles and their individual trajectories with statistical diffusion simulation (DDS) if the conditions of the bulk gas collusions are investigated, the validity, performance, and required modeling effort of these approaches, we designed a relatively simple benchmark problem, and modeled it with both numerical methods. Additionally we build a setup to experimentally verify the theoretical model.

In this contribution we present a detailed comparison and discussion of the numerical and experimental results.

**Methods**

**Numerical Methods**

**Computational Fluid Dynamics (CFD) model**

- Continuous FEM Model (Comsol Multiphysics)

**Discrete particle tracking model**

- SIMION@ with Statistical Diffusion Simulation (DDS) user program

**Discrete particle tracking model**

- Stochastic model / Electrodynamics application model of Comsol Multiphysics v4.0a / v4.1

**Experimental Methods**

**Measurement Chamber**

- Home built sealed chamber with deflection and measurement assembly electrode

**Ions Source**

- Home built corona discharge ion source

**Current Measurement**

- The ion current on the measurement electrode was recorded with our ammeter [Keithley Model 420 electrometer]

**Comparison: Experimental / Numerical Results**

**Ion Migration Simulation Results**

- Continuous FEM Model (Comsol Multiphysics)

**Discrete Model (SIMION / SDS)**

**Benchmark Problem**

- Ions which are produced in a corona discharge ion source are transported into the measurement chamber by gas flow. The gas flow interacts with the charged ions and is pursued out by a rough pump. As a result of the interactions between two electrodes, a detection electrode and a reference electrode, the ion current measured on the detection electrode shows a signal maximum at moderate negative deflection voltage.

**Computational Fluid Dynamics (CFD) Results**

**Figure 3**

- CFD result: Flow velocity magnitude in the chamber, with 1.35 m/s | mean exit gas velocity | 1 bar background pressure. On the left panel, three dimensional flowlines are also drawn.

**Figure 4**

- Dependence of the ion concentration distribution simulated with a continuous ion migration model in Comsol Multiphysics, on the deflection voltage.

- The numerical simulation of the benchmark geometry shows:
  - nearly linear dependencies
  - virtually no interactions between gas flow and electrodes
  - no significant broadening of the gas stream
  - low background ion "leak off" of the gas stream to the outlet port

**Figure 5**

- Dependence of experimentally recorded ion current on the deflection voltage

**Figure 6**

- Theoretical ion current simulated with discrete particle tracking

**Conclusions**

- Both numerical models yield comparable results for the ion trajectories / the ion concentration distribution, respectively.
- Both numerical models qualitatively predict the experimentally determined ion current.
- The SIMION / SDS Model predicts the experimentally found ion current within the modeling and measurement errors, when the estimated ion mobility is corrected appropriately.
- The CFD / SDS Model provides a higher validity level and result quality at much lower numerical costs, as long as the basic assumptions of the SDS method are not violated (no severe space charge).
- The CFD model (used as input data for the ion migration models) is generally the most complex and numerically expensive part of the modeling process.
- The combination of CFD and ion migration models is feasible for the application to more complex problems but experimental validation is generally required.
- If the discrete particle model is not applicable, the higher effort needed for the FEM ion migration model is justified.

**Literature**


- Simion User’s Guide.

- The SIMION / SDS Model predicts the experimentally found ion current within the modeling and measurement errors, when the estimated ion mobility is corrected appropriately.

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