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

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Introduction

In addition to the electrical 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 bulk gas
- **Molecular diffusion** of ions

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

- The **fluid dynamics** 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 (a partial differential equation – PDE) and its numerical solution with the finite element method (FEM)
- Numerical simulation of discrete charged particles and their individual trajectories with statistical diffusion simulation (SDS) [1] of the bulk gas collisions

To investigate the validity, performance and required modeling effort of those 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 models.

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

Methods

Numerical Methods

Computational Fluid Dynamics (CFD) model of bulk gas flow:

"Turbulent Flow" application mode of Comsol Multiphysics v4.0a / v4.1

Discrete particle tracing model:

SIMION v8 with Statistical Diffusion Simulation (SDS) user program, CFD input data from model above, spatial interpolation and conversion of CFD data was performed with home build software

Continuous ion migration model:

"Diluted species" and "Electrostatics" application modes of Comsol Multiphysics v4.0a / v4.1, CFD input from model above

Experimental Methods

Measurement Chamber:

Home built sealed chamber with deflection and measurement electrode assembly

Ion Source:

Home built tubular corona discharge ion source

Ion Current Measurement:

The ion current on the measurement electrode was recorded with a sensitive ammeter (Keithley Model 602 electrometer)

Benchmark Problem

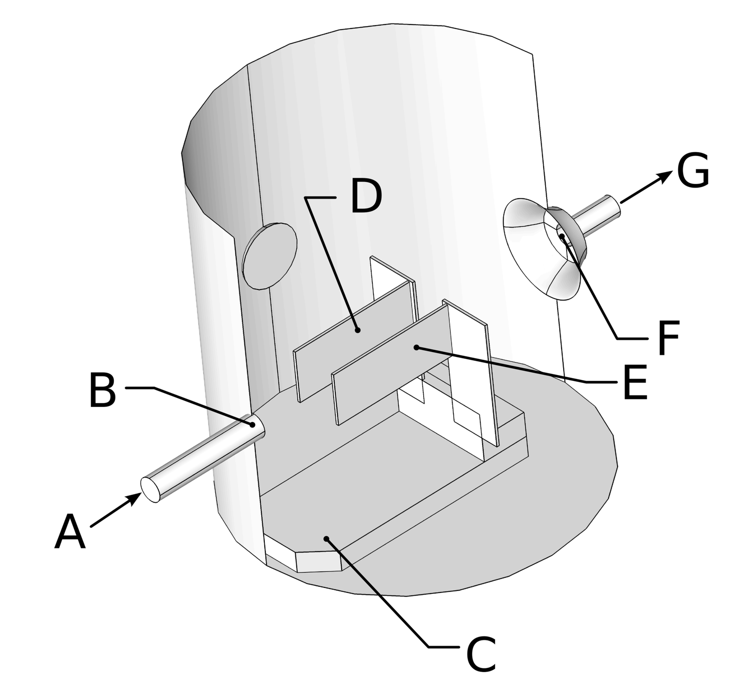

Figure 1) Schematic of the benchmark problem

Ions which are produced in a *corona discharge ion source* are transported into the measurement chamber by a gas flow (**A**). The gas flows trough the chamber and is pumped out by a rough pump (**G**).

It passes between two electrodes, a *deflection electrode* (D) with a variable electrical potential, and a *detection electrode* (**E**).

The experimental result is the dependence of the **ion current measured on the detection electrode** on the gas flow velocity and the deflection voltage.

A: Gas flow from ion source
B: Inlet port
C: Moveable electrode assembly
D: Deflection electrode
E: Detection electrode
F: Outlet port
G: Gas flow to rough pump

Computational Fluid Dynamics (CFD) Results

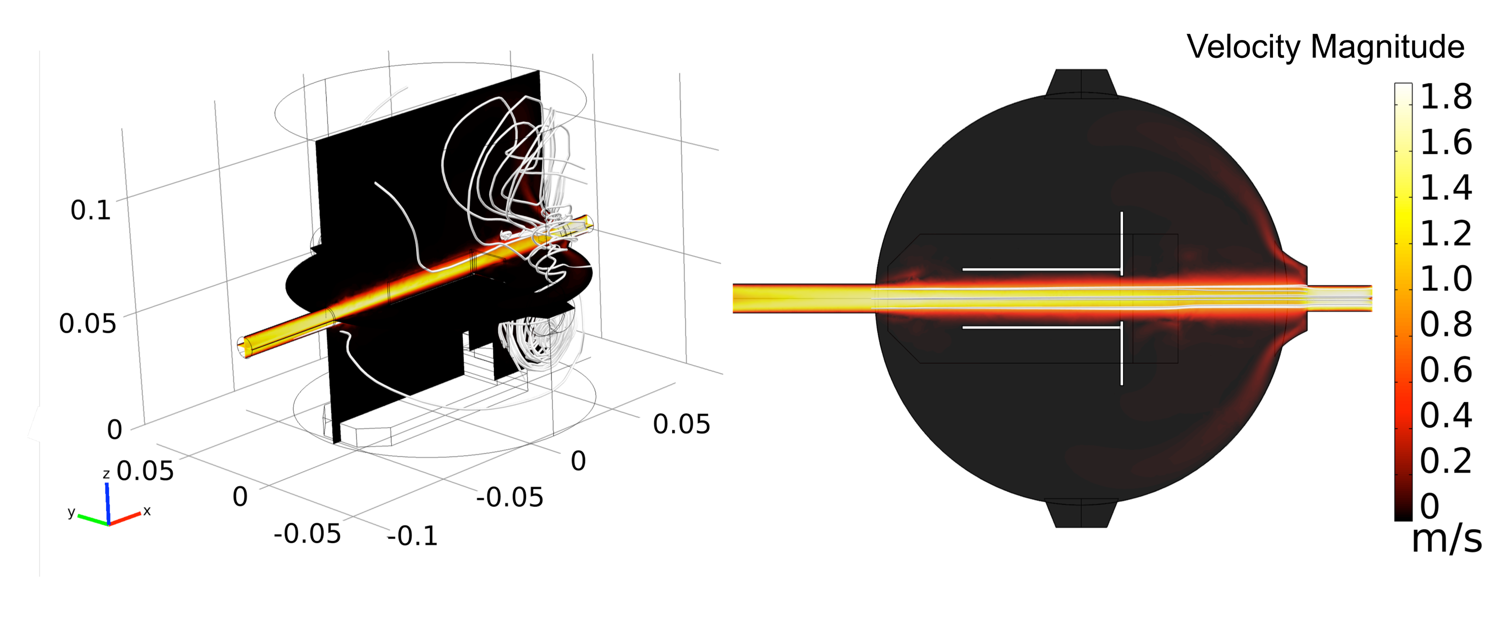

Figure 2) CFD result: Flow velocity magnitude in the chamber, with 1.35 m s^{-1} mean exit gas velocity at 1 bar background pressure. On the left panel, three dimensional flowlines are also drawn

The numerical simulation of the benchmark geometry shows:

- nearly laminar flow conditions
- virtually no interactions between gas flow and electrodes
- no significant broadening of the gas stream
- low backflow / low "peel off" of the gas stream in the outlet port

Ion Migration Simulation Results

Discrete Model (SIMION / SDS)

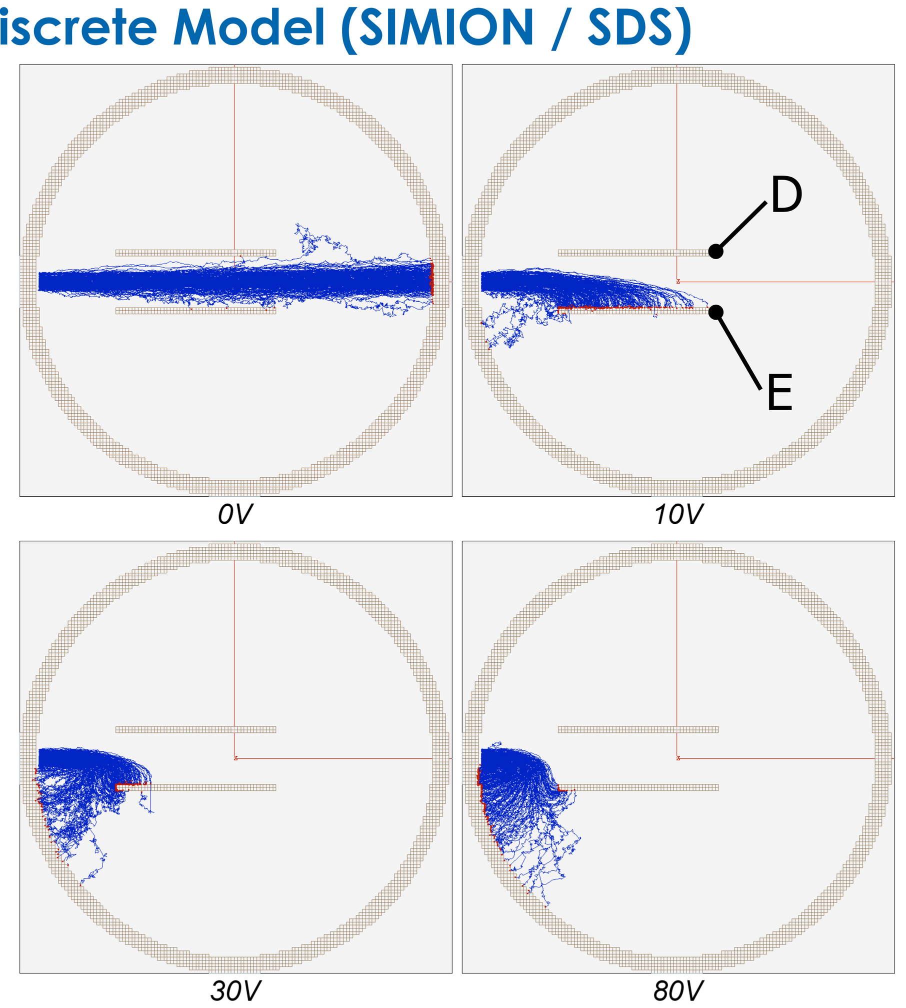

Figure 3) Dependence of ion trajectories simulated with discrete particle tracing (SIMION / SDS) on the deflection voltage

Without deflection potential, the ions are transported only by the viscous drag from the bulk gas flow (**0 V** in *Fig. 3*)

With increasing deflection potential, the ions are pushed out of the gas flow, initially onto the detection electrode (**E** in **10 V** in *Fig.3*); with further increase of the deflection electrode voltage, the electrical forces overcome the viscous drag (**30** and **80 V** in *Fig. 3*)

Therefore the **recorded ion current** on the detection electrode should show a **maximum at moderate deflection voltages**.

Continuous FEM Model (Comsol Multiphysics)

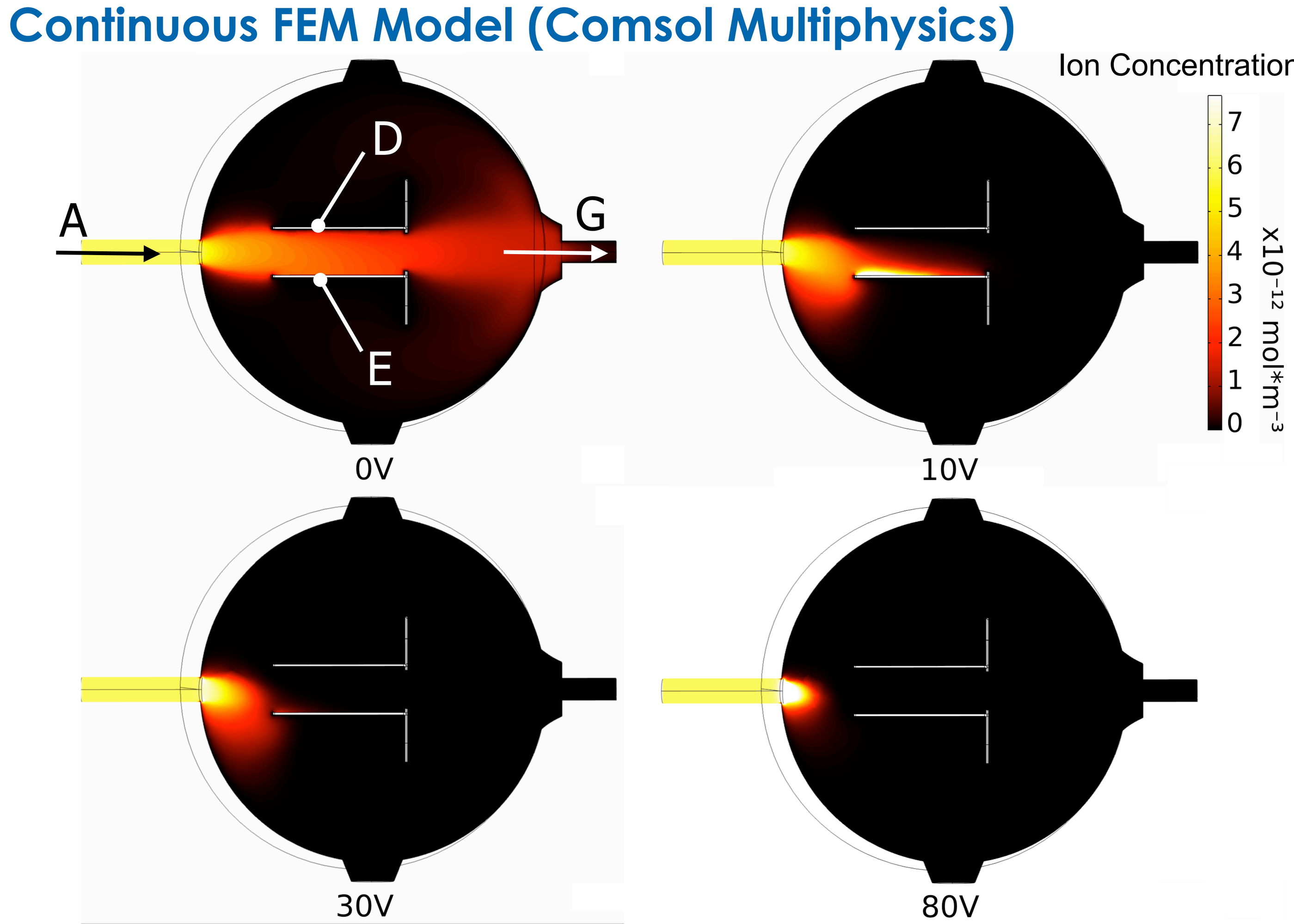

Figure 4) Dependence of the ion concentration distribution, simulated with a continuous ion migration model in Comsol Multiphysics, on the deflection voltage

Basically the FEM Model result is analogous to that of the discrete model:

Without a deflection potential (**0 V** in *Fig.4*) the ions are transported by viscous drag and molecular diffusion.

With increasing deflection voltage, the ion concentration distribution is shifted first onto the detection electrode (**10 V** in *Fig.4*) and then towards the chamber wall (**30** and **80 V** in *Fig.4*).

Experimental Result

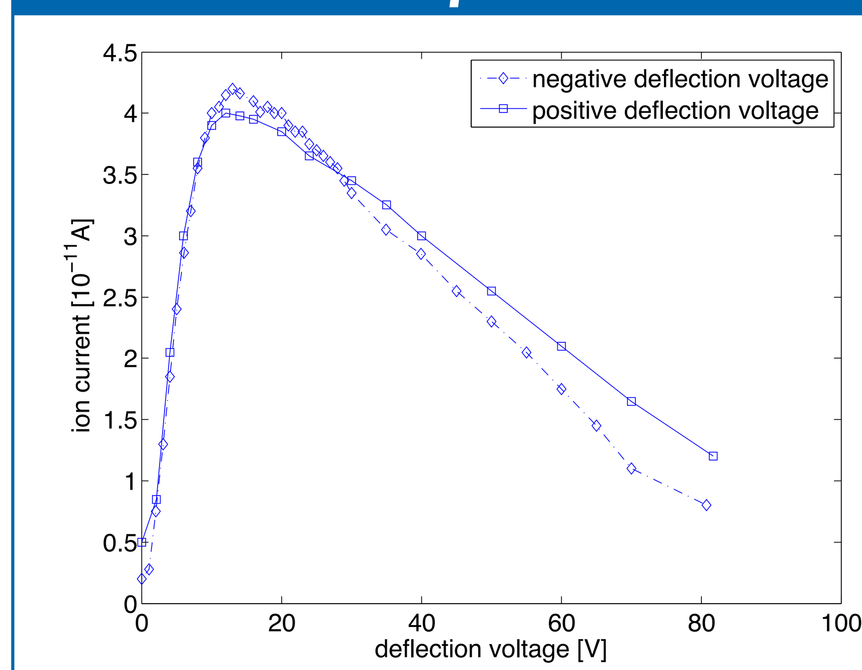

Figure 5) Dependence of experimentally recorded ion current on the deflection voltage

The experimentally measured ion current shows:

- a *mixed ion beam* (note the virtually identical signals with positive and negative deflection voltage)
- a signal maximum at ~20V deflection potential, which was qualitatively predicted by the numerical models (cf. *Fig 3* and *Fig. 4*)

Comparision: Experimental / Numerical Results

Discrete Model

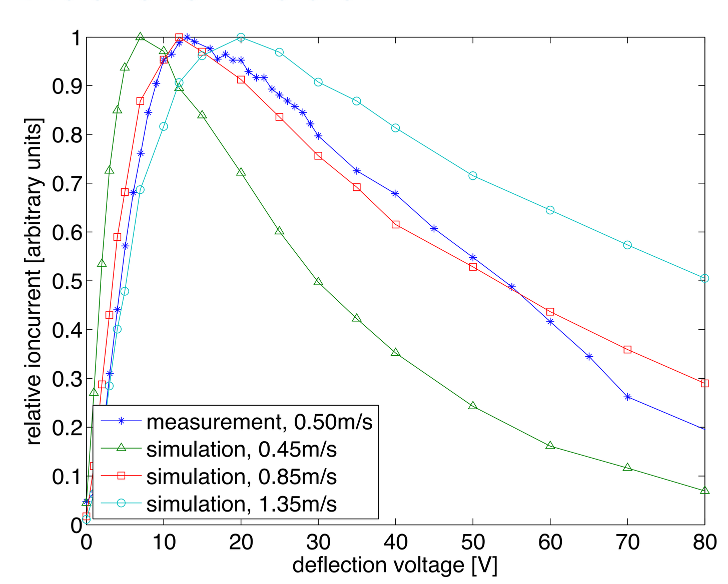

Figure 6) Theoretical ion current simulated with discrete particle tracings

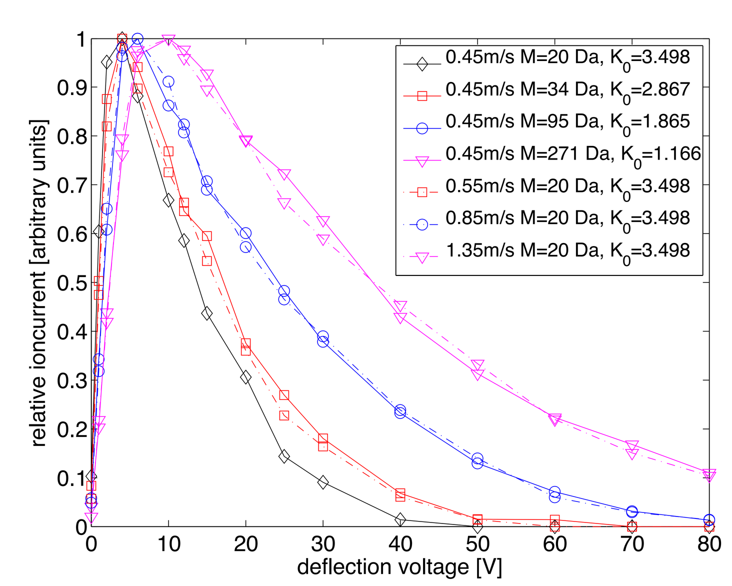

Figure 7) Inverse effects of the gas velocity and the ion mobility in the discrete model, the ion mobility K_0 is given in units of $10^{-4}\,m^2\,V^{-1}\,s^{-1}$

Continuous FEM Model

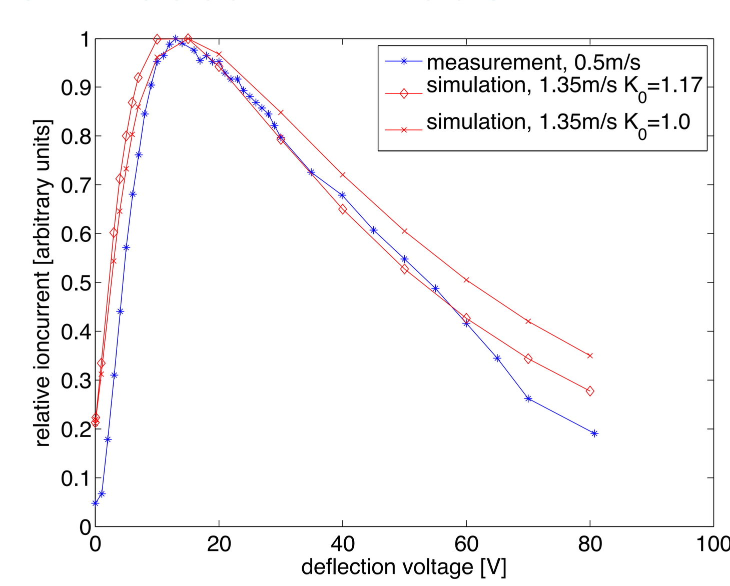

Figure 8) Theoretical ion current simulated with the continuous FEM model, the ion mobility K_0 is given in units of $10^{-4}\,m^2\,V^{-1}\,s^{-1}$

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 SIMION / 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

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Acknowledgement

Financial support is gratefully acknowledged:
DFG (BE2124/6-1 and BE2124/4-1)