Modular computational toolset for atmospheric pressure ionization method development: SIMION meets FEM

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Introduction

The numerical simulation of ion trajectories under collision free conditions using the program package SIMION has matured into a very powerful tool for ion optics and mass analyzer development.

Unfortunately ion trajectory calculations at elevated or even atmospheric pressure are disproportionately more difficult. At such high pressures, the motion of charged particles is governed not only by electrical fields but also by fluid-dynamical forces.

Thus the numerical simulation of the fluid dynamical conditions in the high-collision rate areas of a device appears to be a prerequisite for meaningful ion trajectory calculations.

In addition, at high collision rates chemical transformations of charged particles (ion-molecule reactions) potentially alter the primary generated ion distribution.

Towards this end we have developed a modular toolset for the numerical simulation of ion motion and transformation under elevated pressure by combining existing software packages.

Modular Toolset

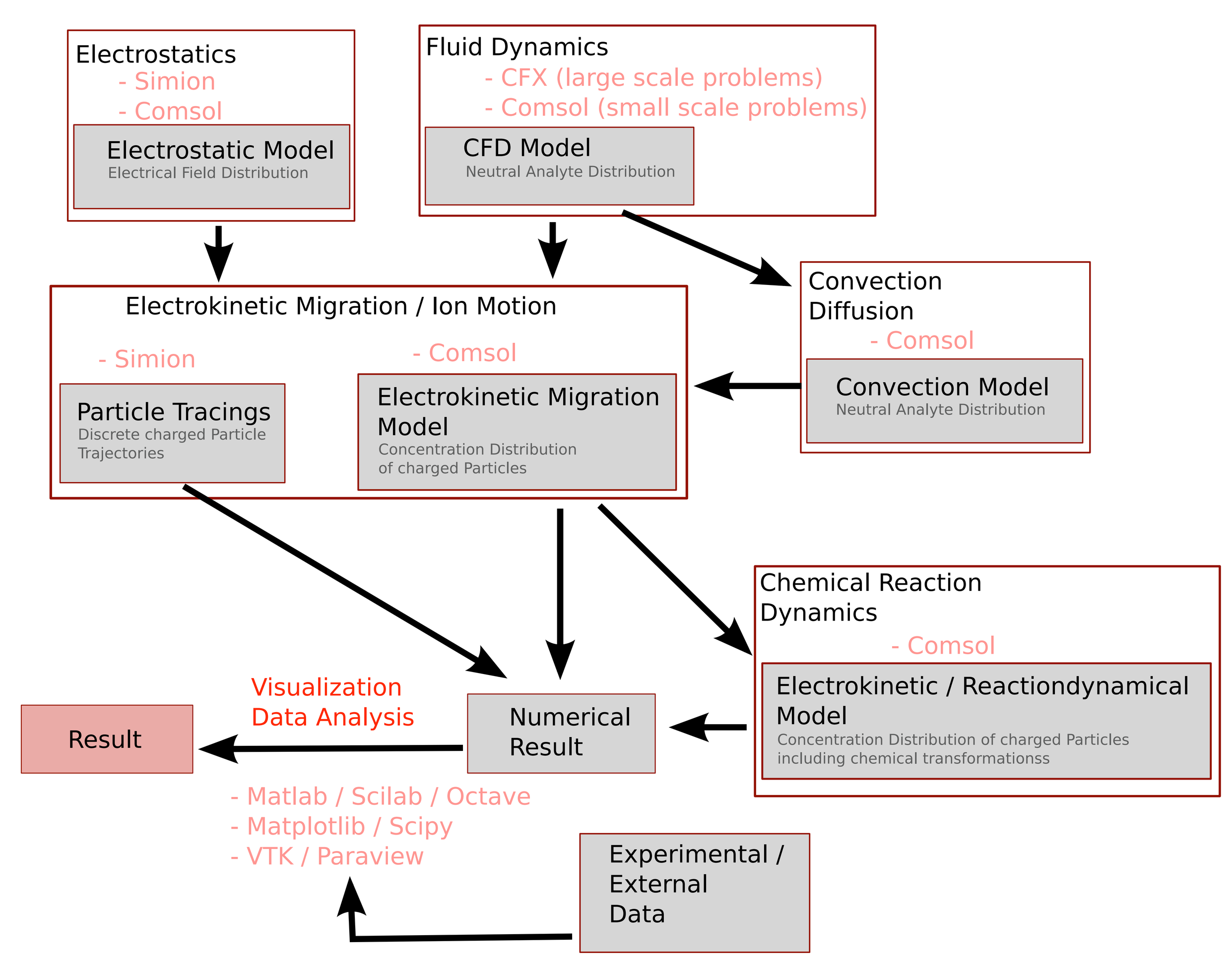

Fig. 1: Toolset Overview

Problem driven choice of tools:

- The configuration of the solver / visualization pipeline is fully governed by the problem under investigation

- The toolset contains two numerical solvers for the charged particle motion:
  - **SIMION 8** (with SDS Algorithm[1]) using a *discrete, particle tracing* approach
  - **COMSOL Multiphysics 3.4a** with a *continuum electrokinetic* approach
- Fluid dynamic input data for the solvers were generated with **Ansys CFX** and **COMSOL Multiphysics**
- Visualization and calculation result analysis was performed using closed source (Matlab) and open source tools (VTK / Paraview, Scipy / Matplotlib, Scilab)

Transfer Capillary Outflow

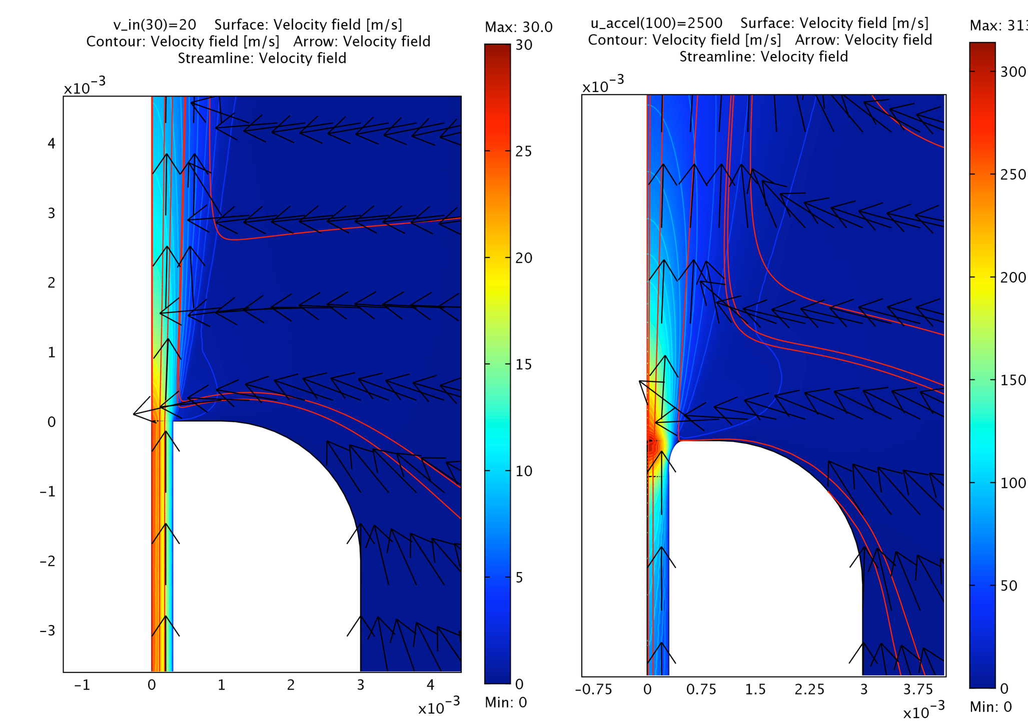

Fig. 2: COMSOL Simulation of the outflow of a transfer capillary at 800 mbar (left) and 4 mbar (right) background pressure

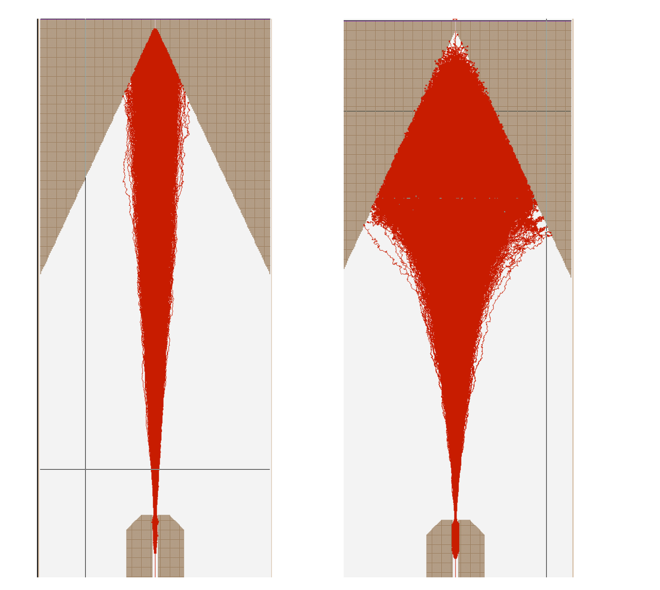

Fig. 3: SIMION Simulation of the ion motion in the transfer capillary outflow, with 500V acceleration voltage at 800 (left) and 4 (right) mbar background pressure

- Problem to solve was the motion of ions in the outflow of a transfer capillary into a given recipient geometry with variable background pressure (see poster *WP 609* for further details)
- Fluid dynamical models for different pressures were solved using COMSOL (Fig. 2)
- Fluid flow solutions were used for discrete particle tracing (see Fig. 3) calculations with Simion
- Simion was also used for simulating the time of flight distribution of ion packages within the referenced geometry under different conditions (not shown)

Conclusions

- A modular computational toolset for ion trajectory simulations at high neutral collisions rates (i.e. elevated pressure up to 1 atm) was developed
- First multiphysical numerical models were successfully solved and experimentally verified
- The results presented and the application of these tools in our current research regarding the performance increase of API sources clearly show the feasibility of the chosen approach
- Even complex geometries such as existing commercial API sources with multiple gas flow sources and sinks were successfully modeled
- In the near future, largely computer aided API source design appears to be feasible

Ion Motion in tubular APCI Source

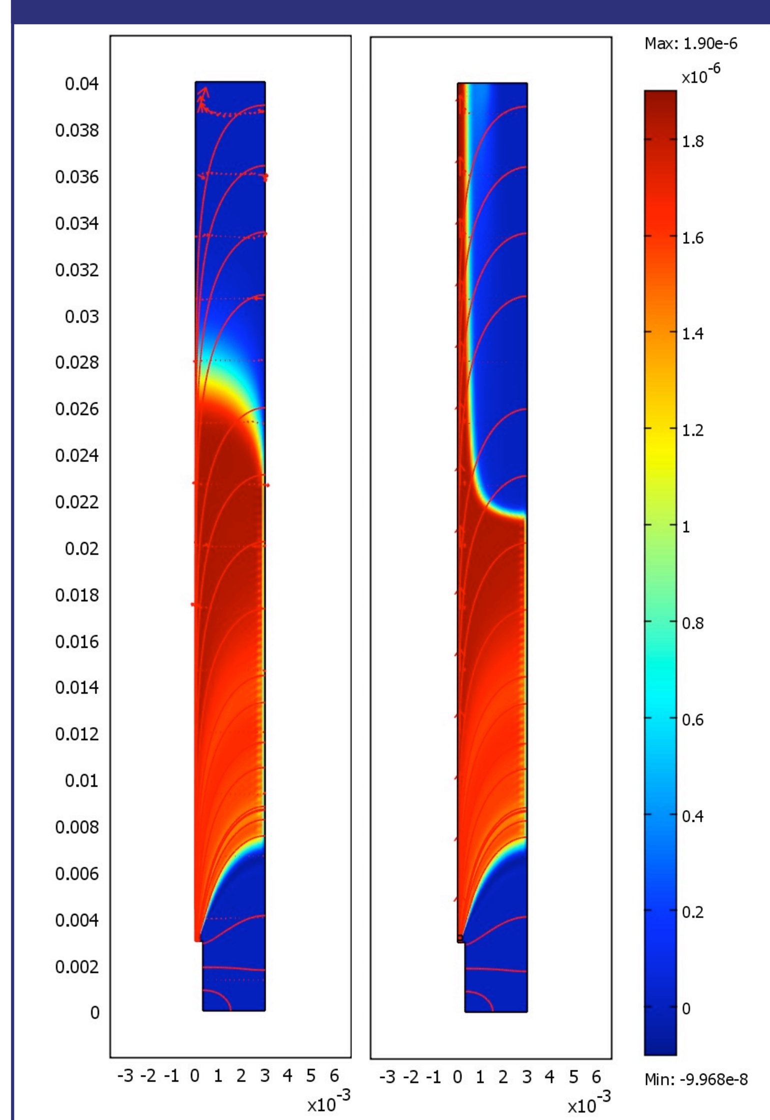

Fig. 4: COMSOL Simulation of the electrokinetic ion motion in a tubular APCI ion source without gas inflow (left) and 0.45l/min gas inflow (right) for 2000V APCI Needle voltage

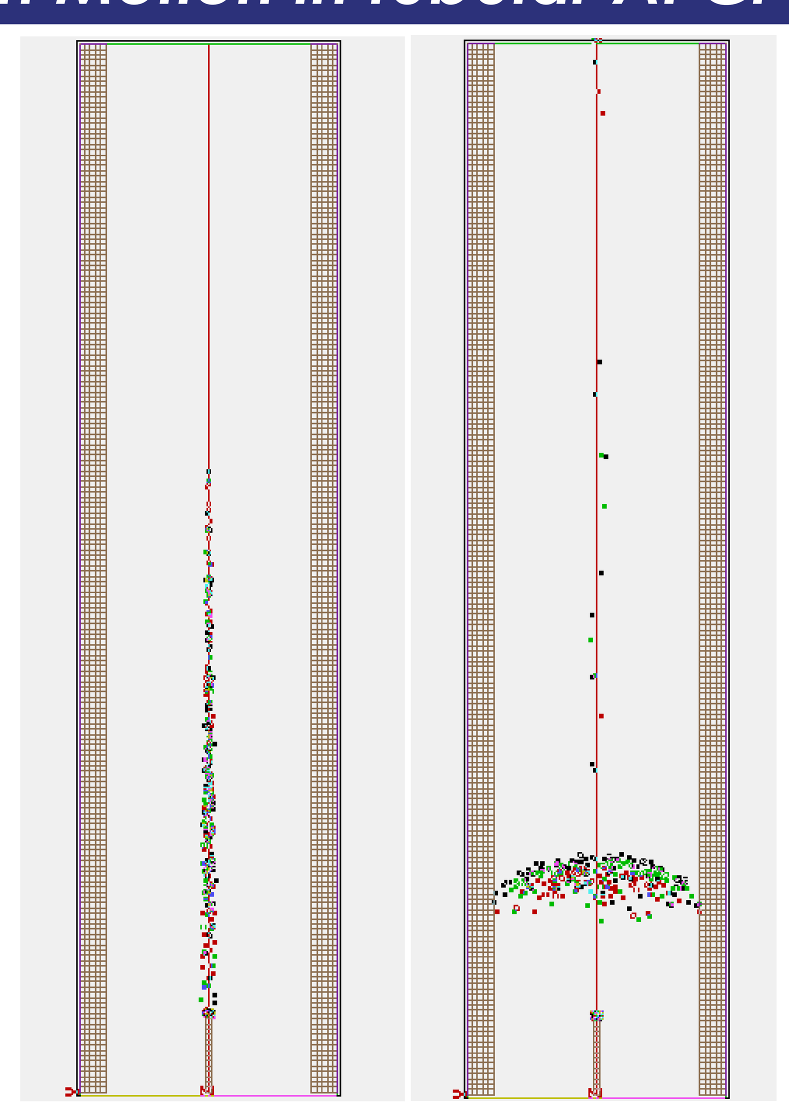

Fig. 5: Charged particle motion simulated with Simion in a tubular APCI ion source, without (left) and with (right) high voltage (2000 V) on the APCI corona needle

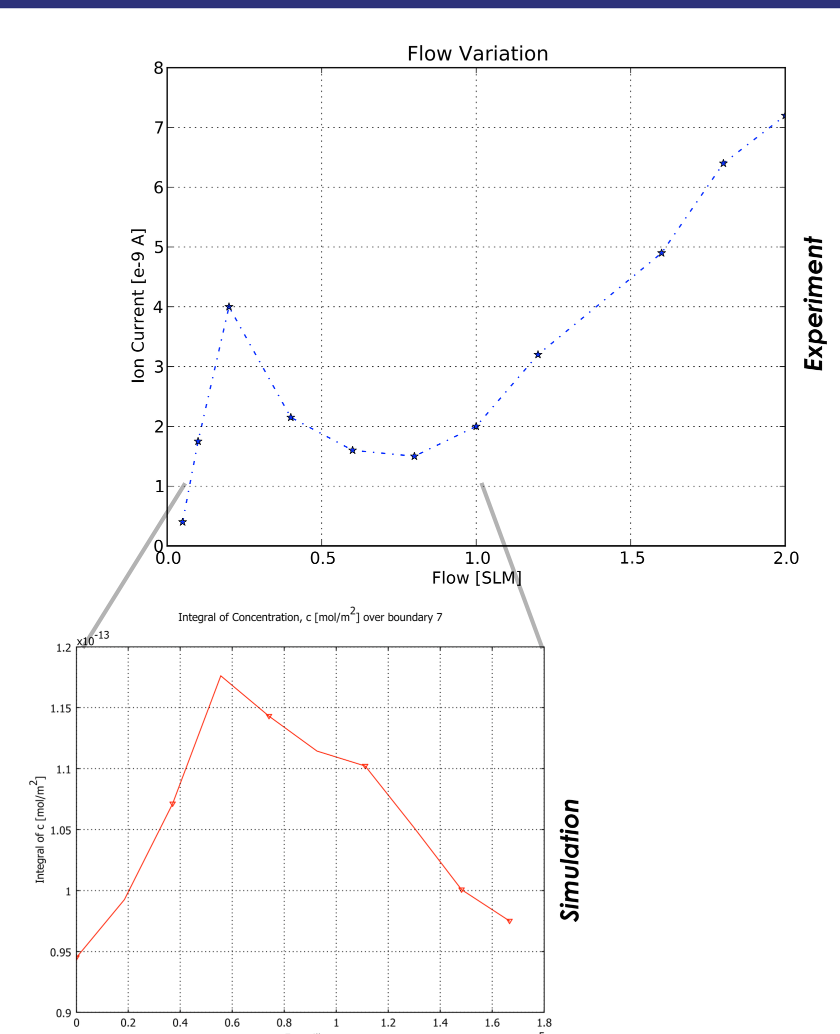

Fig. 6: Comparison between simulated and experimentally measured ion current out of a tubular APCI ion source

- Problem to solve was the motion of ions in a tubular APCI ion source
- Fluid dynamical models were solved using COMSOL
- Fluid flow solution was used for electrokinetic (see Fig. 4) and particle tracing (see Fig. 5) calculations
- Models were compared with experimental data (Fig. 6)

Complex Fluid Dynamics in AP Ion Source and Validation

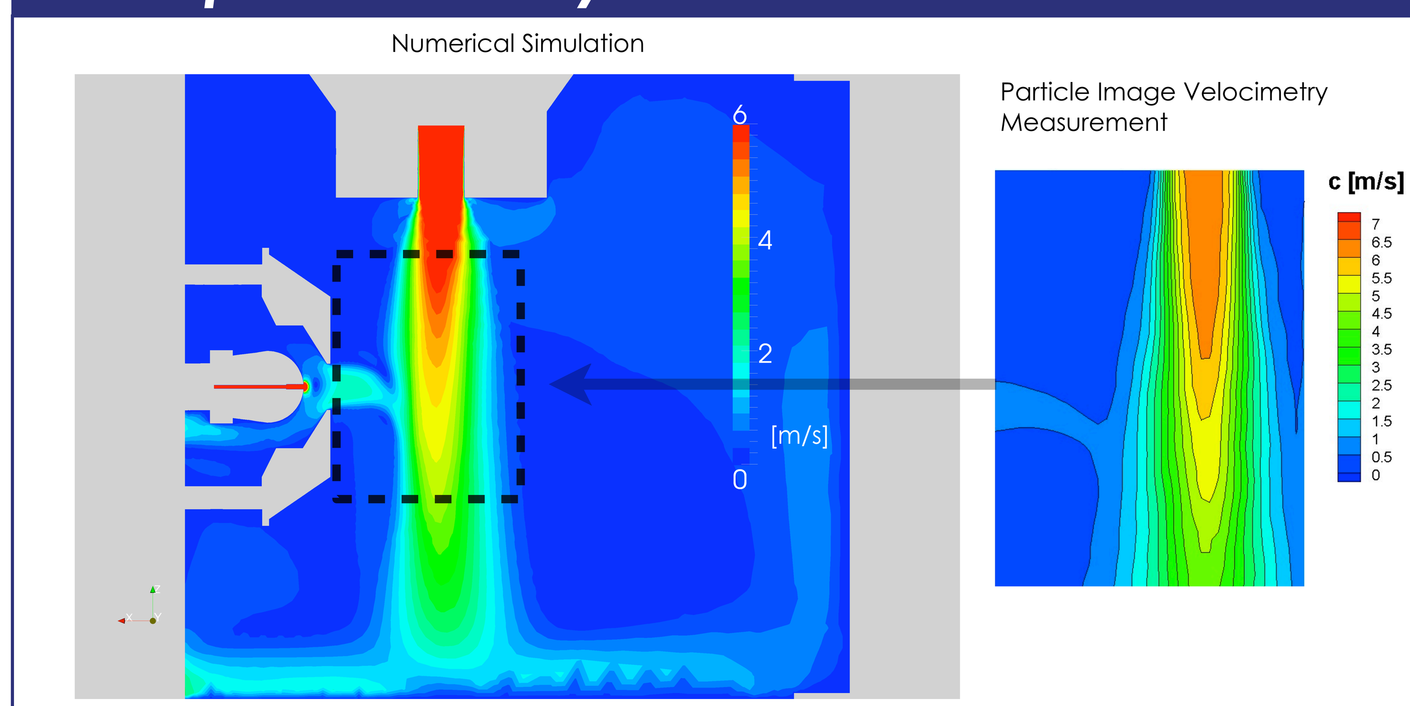

Fig. 7: Numerical simulation (using Ansys CFX) and Particle Image Velocimetry (PIV) measurement of the complex fluid dynamic conditions inside an AP Ion source

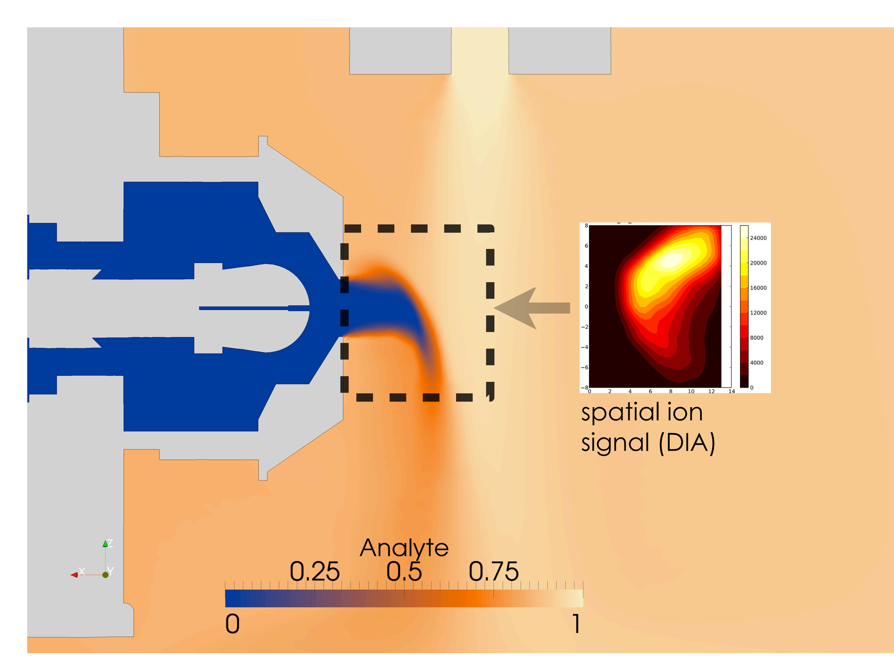

Fig. 8: Convective neutral analyte distribution (modeled using Ansys CFX) and spatially resolved ion signal recording (DIA)

The fluid dynamical conditions in AP ion sources can be very complex. The shown numerical model was derived with Ansys CFX on a high performance cluster computer.

Top:

The numerical simulation (top left) of the complex fluid dynamics in the AP ion source and the experimental Particle Image Velocimetry (PIV) data (top right) clearly demonstrates the validity of the numerical model

Left:

The neutral analyte distribution in the AP Ion source strongly suggests the lack of suitable neutral analyte concentration as reason for the minimum in ion signal intensity directly in front of the MS inlet. Spatial resolved ion tracing calculations would allow verification of this explanation; this is work in progress.

See poster WP 610 and Reference 4 for details on spatial resolved ion signals (Distribution of Ion Acceptance, DIA).

References

1) Anthony D. Appelhans, David A. Dahl; *SIMION ion optics simulations at atmospheric pressure*, Int. J. Mass spectrom., Vol. 244, **2005**, 1-14
2) David A. Dahl, Timothy R. McJunkin, Jill R. Scott; *Comparison of ion trajectories in vacuum and viscous environments using SIMION: Insights for instrument design*; Int. J. Mass spectrom., Vol. 266, (1-3), **2007**, 156-165
3) Sebastian Barth, Stefan Zimmermann, Modeling Ion Motion in a Miniaturized Ion Mobility Spectrometer, Proceedings of the COMSOL Conference **2008**, Hannover, Germany
4) Matthias Lorenz, Ralf Schiewek, Klaus J. Brockmann, Oliver J. Schmitz, Siegmar Gäb, Thorsten Benter; *The Distribution of Ion Acceptance in Atmospheric Pressure Ion Sources: Spatially Resolved APLI Measurements*, J. Am. Soc. Mass. Spectrom., Vol. 19, (3), **2008**, 400-410
5) Walter Wißdorf, Matthias Lorenz, Hendrik Kersten, Sonja Klee, Klaus J. Brockmann, Thorsten Benter; Atmospheric Pressure Laser Ionization (APLI): Systematic DIA Measurements for APLI Method Development, Poster presented at the 57th ASMS annual meeting, May **2009**, Philadelphia, USA

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