Numerical Simulation of the Distribution of Ion Acceptance (DIA) in a Commercial API Source

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Introduction

The spatial resolved ion signal distribution in an ion source was introduced [1] as **Distribution of Ion Acceptance** (DIA). Under atmospheric pressure conditions, this distribution depends on the electrical field, the bulk gas flow, the distribution of the neutral analyte and chemical reactions occurring in the ion source.

In the recent past we thoroughly investigated the impact of various parameters of an commercial AP ion source on the DIA with experimental methods (experimental DIA measurements, with APLI [2]) and gained a much better understanding of the conditions prevailing inside the source geometry [3]. However, the observed DIA is a complex and highly convoluted data set, which incorporates all dependencies of the ion motion simultaneously. Thus the DIA does not provide a direct insight into the internal dynamics of an AP ion source and the interpretation of DIA is rather difficult.

With the recent advances in numerical simulation method development, the simulation of ion migration under complex conditions, and therefore the simulation of DIA, became feasible (see also Poster 070 in session TP04).

The numerical simulation of DIA and comparison with experimental DIA data allows the verification of the entire numerical ion migration model.

In addition, an experimentally verified numerical model provides a detailed insight into the dynamical processes in the ion source, which would not be achievable with experimental methods.

In this work we show a numerical model for the distribution of ion acceptance in a commercial AP ion source and compare the numerical results with experimental DIA data.

Methods

Numerical Methods

Discrete ion migration model:

- SIMION v8 with Statistical Diffusion Simulation (SDS)
- Fluid dynamic data are provided from a detailed computational fluid dynamics (CFD) model of the ion source (CFD Solver: Ansys CFX v.12.1, see poster 069 in session TP04 for details)

Data analysis / Visualization / SIMION automation:

- The automation of the ion migration model was performed with self developed scripts, implemented in the python programming language
- The data analysis and visualization of the result was also performed with customized python scripts, for this task the Matplotlib, Numpy and Scipy Python libraries were used

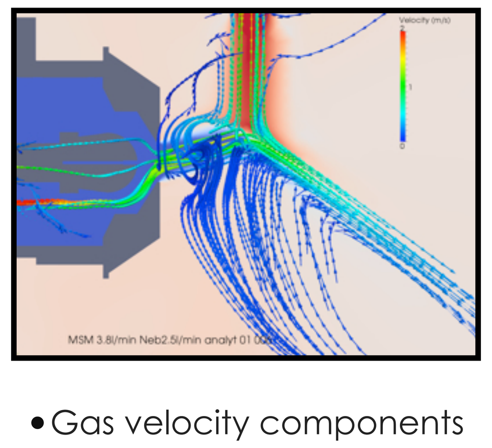
Experimental Methods

Laser system:	ATL ATLEX 300 SI, KrF*; λ = 248 nm 3 mJ/pulse 4 … 8 ns pulse duration 100 Hz pulse frequency
Beam delivery:	Computer-controlled 2-way beam positioning stage
Mass analyzer:	Bruker micrOTOF with a multi-purpose ion source (MPIS[8])
Analyte Solution:	1 µmol/l Pyrene in methanol
Injection Parameters:	Direct injection via HPLC pump with 100 µl/min liquid flow

Simulation Process

CFD Input

Ansys CFX 12.1



- Gas velocity components
- Pressure distribution
- Temperature distribution
- Neutral Analyte distribution

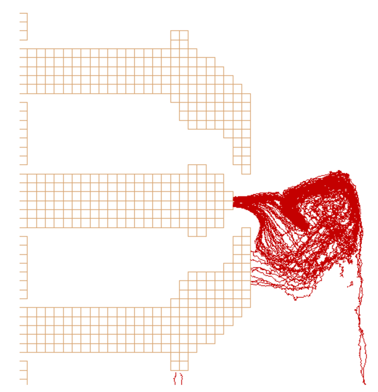
Spatial Interpolation

proprietary
(Matlab)

CFD Data on the irregular discretization mesh must be interpolated for the rectangular mesh of SIMION

Ion Trajectory Simulation

SIMION 8 / SDS
Automation, proprietary
(Python, SciPy, NumPy)



- For every spatial positon of the DIA dataset a "bunch" of ions is started
- The number of flown ions is scaled by the neutral analyte distribution (max. 5000 ions per position, ~2500 spatial positions)

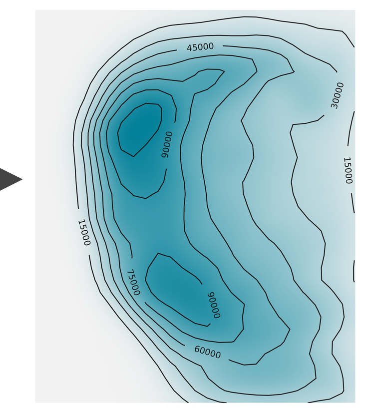
Data Analysis

proprietary
(Python, SciPy, NumPy)

the trajectories terminating on the MS inlet capillary are considered "successful"

Simulated DIA

Visualization, proprietary
(Python, Matplotlib, VTK)



- The result is a simulation of the DIA
- It is simulated with resolution in all 3 dimensions
- Comparison with experimental DIA data after projection on a plane

The DIA in the MPIS

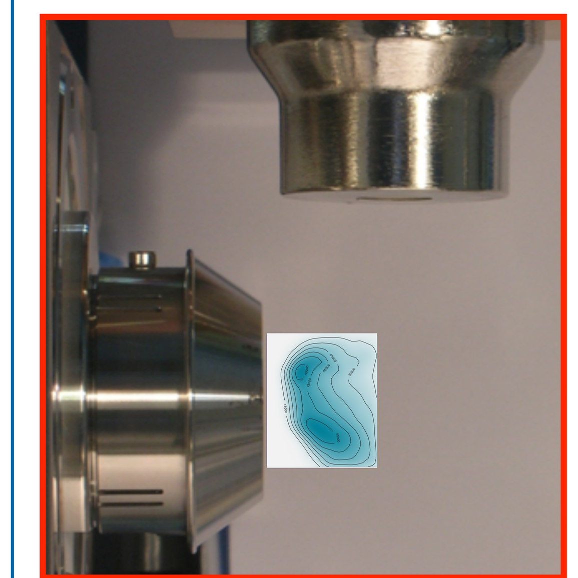


Figure 1) Position of DIA in the multi purpose ion source (MPIS)

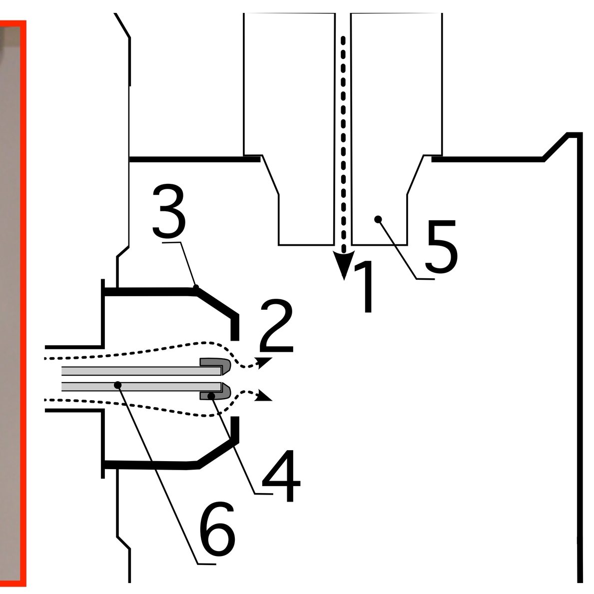


Figure 2) Schematic of MPIS
1: Nebulizer Gas **2:** Dry Gas **3:** Sprayshield **4:** Capillary Cap **5:** Nebulizer **6:** MS Inlet Capillary

Results

Sprayshield Voltage Variation at **500V** Capillary Voltage

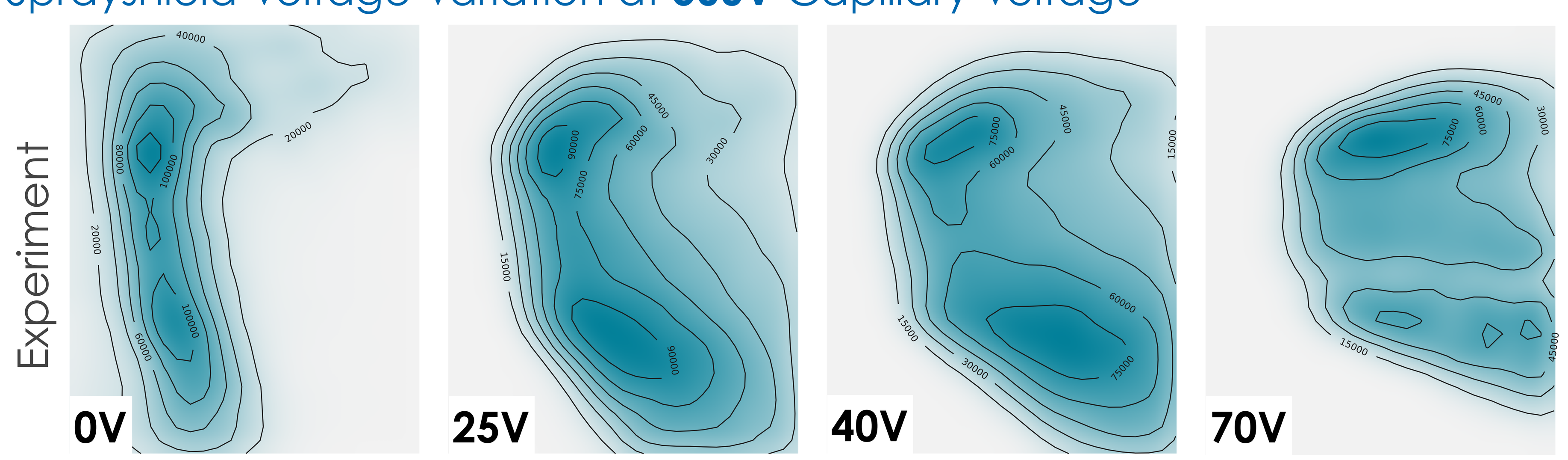


Figure 3) DIA measurements with a Capillary Voltage of 500V (4 in Fig. 2) and variation of the Sprayshield Voltage (3 in Fig. 2)

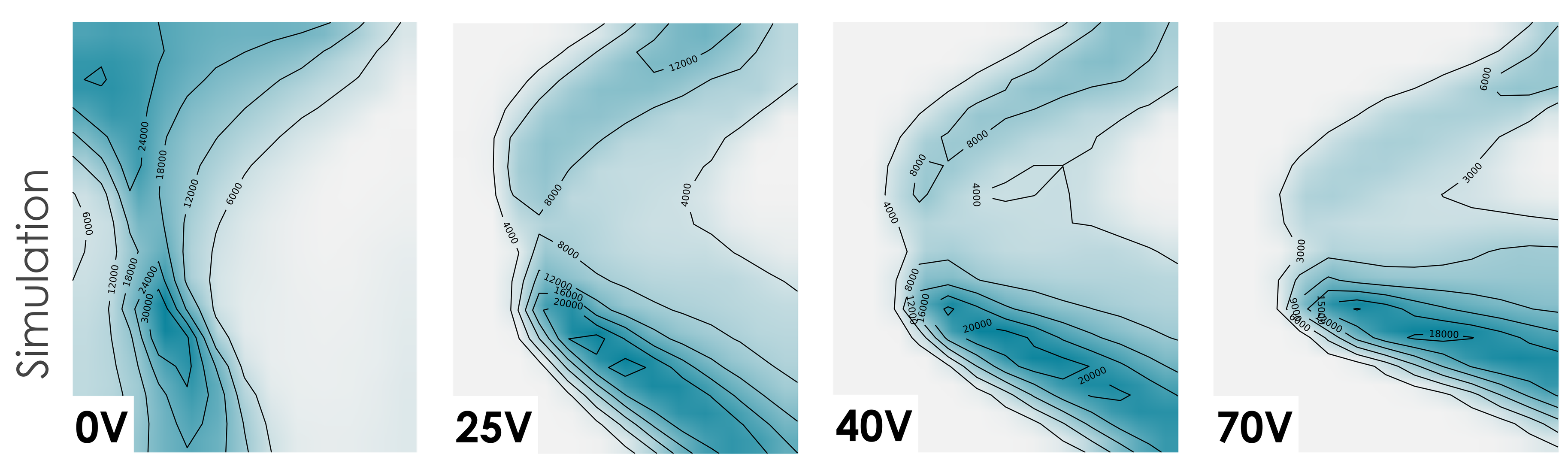


Figure 4) Numerical simulations of the measurements shown in Fig. 3, here a projection of the full 3d dataset is shown

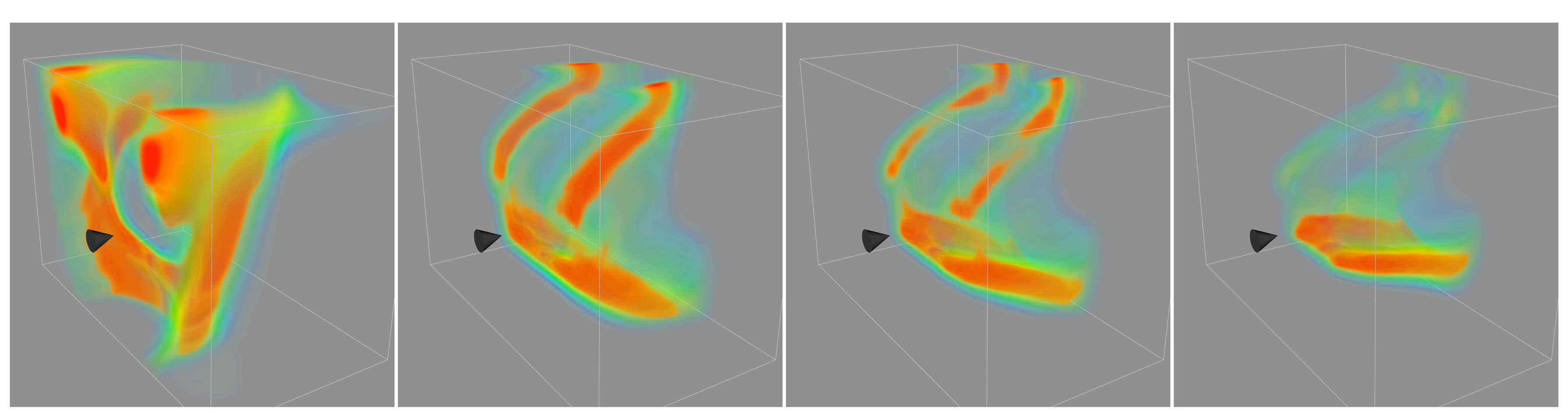


Figure 5) 3d representation of the simulated DIA shown in Fig. 4, the position of the capillary is marked with the dark cone

Sprayshield Voltage Variation at **1000V** Capillary Voltage

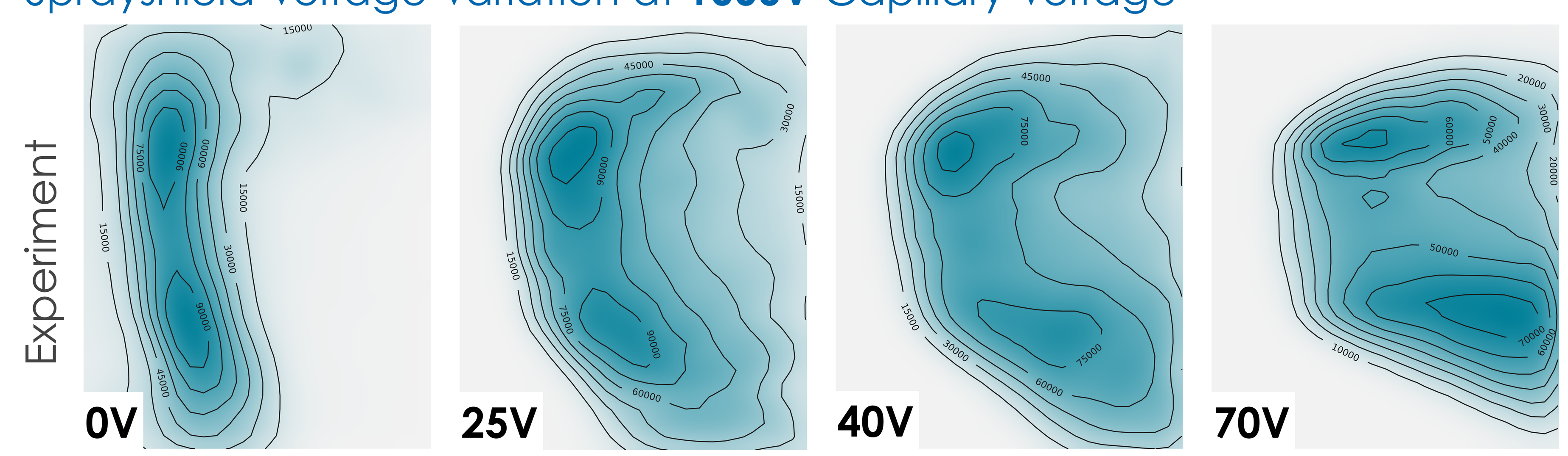


Figure 6) DIA measurements with a Capillary Voltage of 1000V (4 in Fig. 2) and variation of the Sprayshield Voltage (3 in Fig. 2)

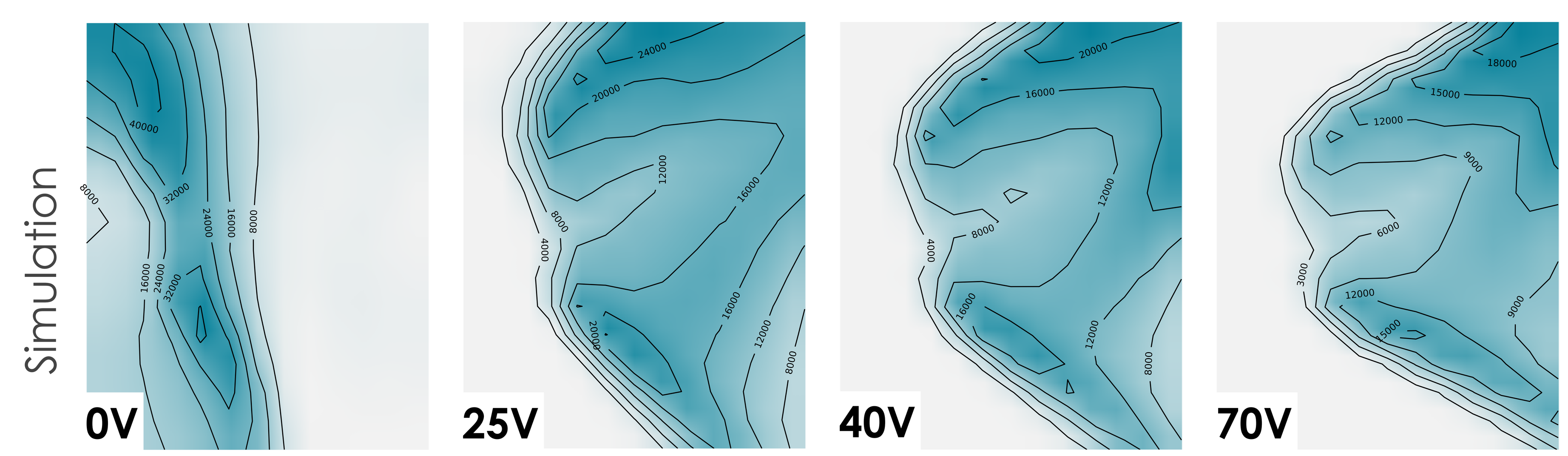


Figure 7) Numerical simulations of the measurements shown in Fig. 6, here a projection of the full 3d dataset is shown

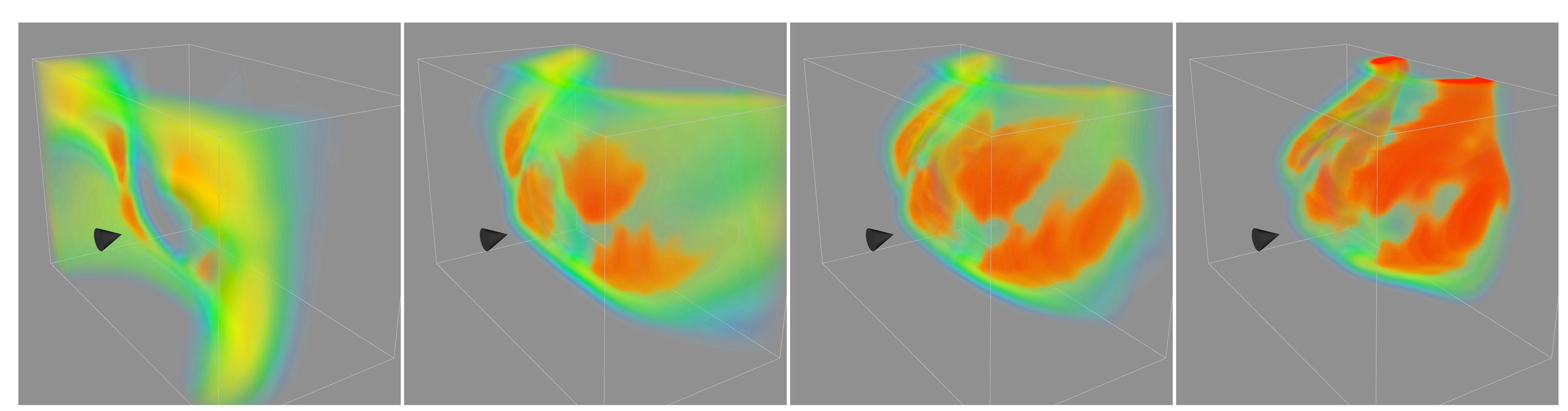


Figure 8) 3d representation of the simulated DIA shown in Fig. 7, the position of the capillary is marked with the dark cone

Conclusions

- Good qualitative agreement between numerical simulation and experimental results (Fig. 3,4 / 6,7)
- All important features of the experimentally determined DIA are reproduced in the simulations:
  - Signal minimum in front of MS capillary
  - Signal minimum on center axis
  - Dependence on the variation of the sprayshield voltage
- Results show general feasibility of simulation approach: Ion trajectory tracings with SIMION / SDS based on numerical CFD input data yield reasonable results, even under very complex conditions
- The numerical model yields results which are not yet experimentally available (three dimensionally resolved DIA, cf. Fig. 5 and 8)
- Particle calculations and data analysis is performed on advanced standard computer hardware ("Workstation" Class PC)
- A numerical model driven ion source development process is possible but requires a valid CFD model of the ion source, which is the numerically most expensive part of the entire simulation process

Literature

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