Simulation of the pressure dependent Dynamic Ion Acceptance Volume (DIAV) of an electrically biased external ion sampling stage

BERGISCHE UNIVERSITÄT WUPPERTAL

Physical & Theoretical Chemistry
Institute for Pure and Applied Mass Spectrometry
University of Wuppertal

Markus Hübner*, Sanna Benter, Laura Lehmann, Hendrik Kersten, Thorsten Benter
*ralf.huebner@uni-wuppertal.de

Introduction

Sampling efficiency is a major consideration in the design of most mass spectrometric measurements. Unfortunately, this collides with another requirement, when sampling ions directly from a (moderately) pressurized vacuum recipient: The desired pressure gradient towards the ion transfer stage / the mass spectrometer is often accomplished by use of a restrictor electrode with a small aperture, which - despite its ion guiding function - limits the amount of ions transferred into the MS system.

In this work, the spatially resolved sampling efficiency of a lens system with a smallest entrance orifice radius of 0.25 mm is examined, which serves as the separator between a plasma region and the transfer system of a high-resolution time-of-flight mass spectrometer (**TOF-MS**). A strong dependence of transmission efficiency for these ions on initial position is expected. This study aims to quantify the sampling efficiency of the aforementioned setup with respect to background gas pressure and initial ion kinetic energy.

Methods

Simulations were carried out at 1 and 2 Pa plasma chamber, respectively, and for variable ion kinetic energy. The sampling efficiency was visualized in relative terms in a discretized spawn area.

SIMION[1]

- Calculation of H_3^+ ion trajectories
- Hard-sphere collision model
- Tracking of "survivors"

PICLas[2]

- Particle in cell and DSMC based plasma simulation software
- No variation of parameters
- Simulation of H_2^+ ions
- Inclusion of space charge effects (Poisson solver)

Mesh for PICLas

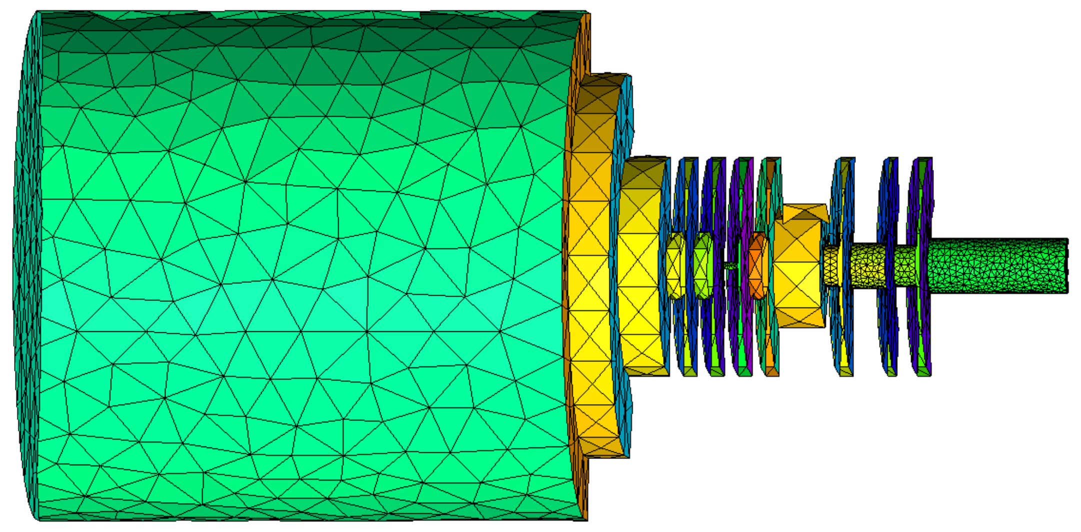

Figure 2: Cross section of the mesh used for PICLas simulation (only surface elements shown for clarity)

PICLas Results

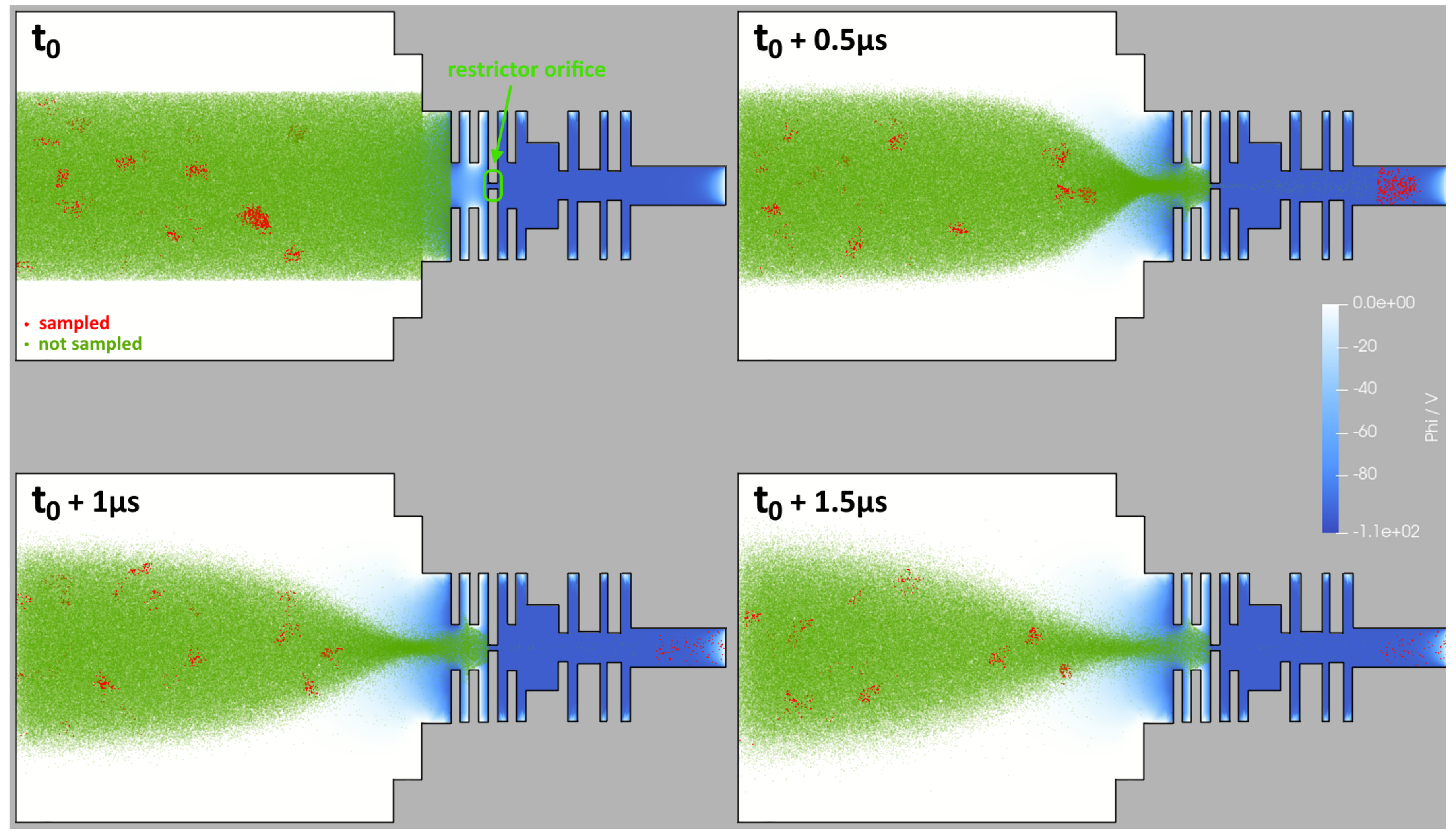

Figure 3: Simulated results in PICLas: sampled ions in red, electric potential heat map

- Most ions impact on the restricting electrode
- Clustered initial positions as sampling or simulation artefact
- No relevant impact of space charge at the simulated ion densities was found

Simulation Setup

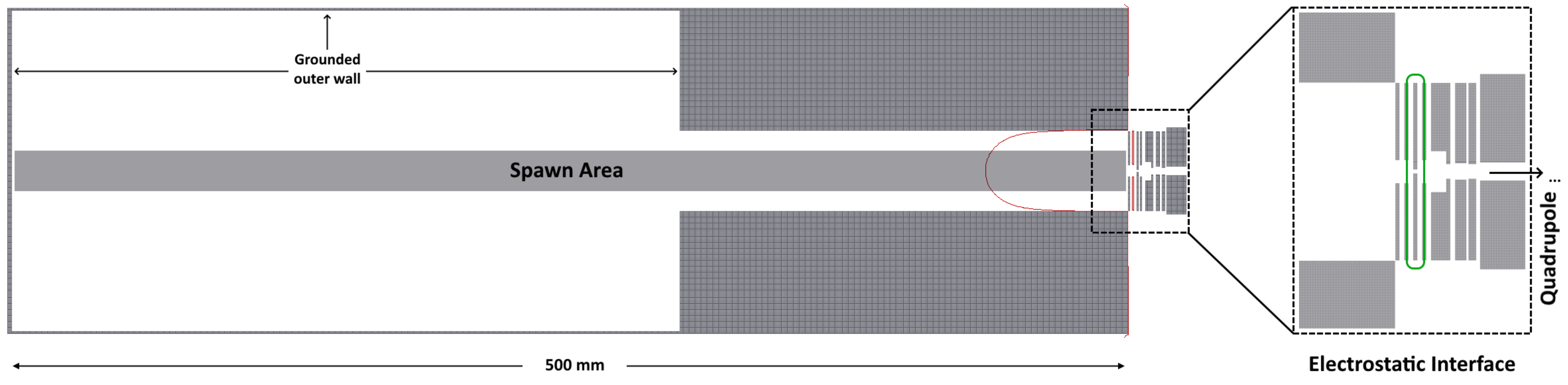

Figure 1: Simulation domain with 0.03 V equipotential line (red, referring to thermalized ions) and electrostatic interface with the restrictor (green) and dummy quadrupole; ions were spawned inside the gray area

- Approximated experimental configuration via SIMION and gmsh[3] (for PICLas)
- Rotationally symmetrical geometry
- Zero-potential boundaries greatly shape the hyperpotential surface
- Ions reaching the "dummy quadrupole" were considered as successfully sampled

SIMION: 1) Kinetic Energy Dependence

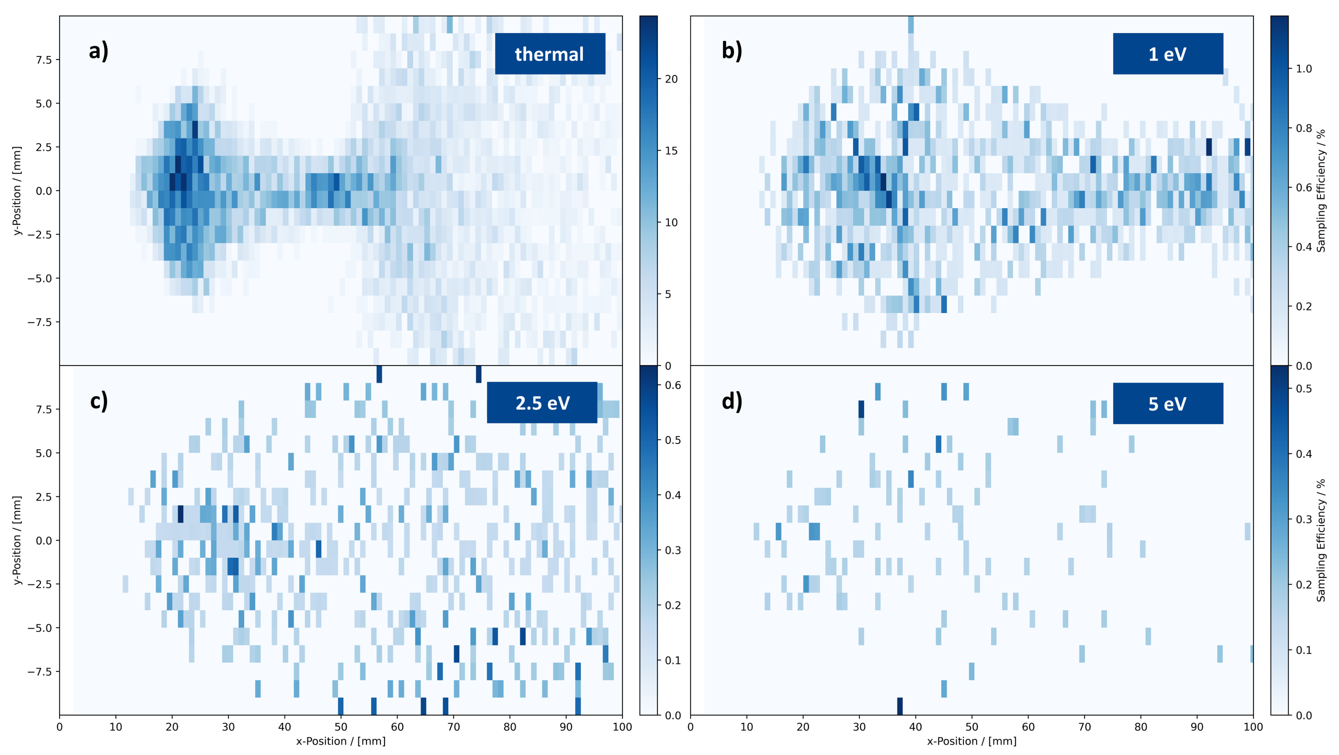

Figure 4: Transmission efficiencies for different starting velocity distributions

No significant difference was found between the calculations at 1 and 2 Pa, respectively.

The probability of successful sampling for any given ion exhibits a strong dependence on both initial position and kinetic energy, as expected. The 2D-histogram in **Figure 4a** reveals a distinct shape for the bulk region of sampled ions, which is theorized to be the projection of the hyperpotential surface of the interface with regard to transmission. For higher starting energies, this shape becomes increasingly blurred, which is in accordance with the theory that the phase space of sampled ions is mainly determined by the electrostatic landscape created by the lens stack.

2) Flight Time Profile

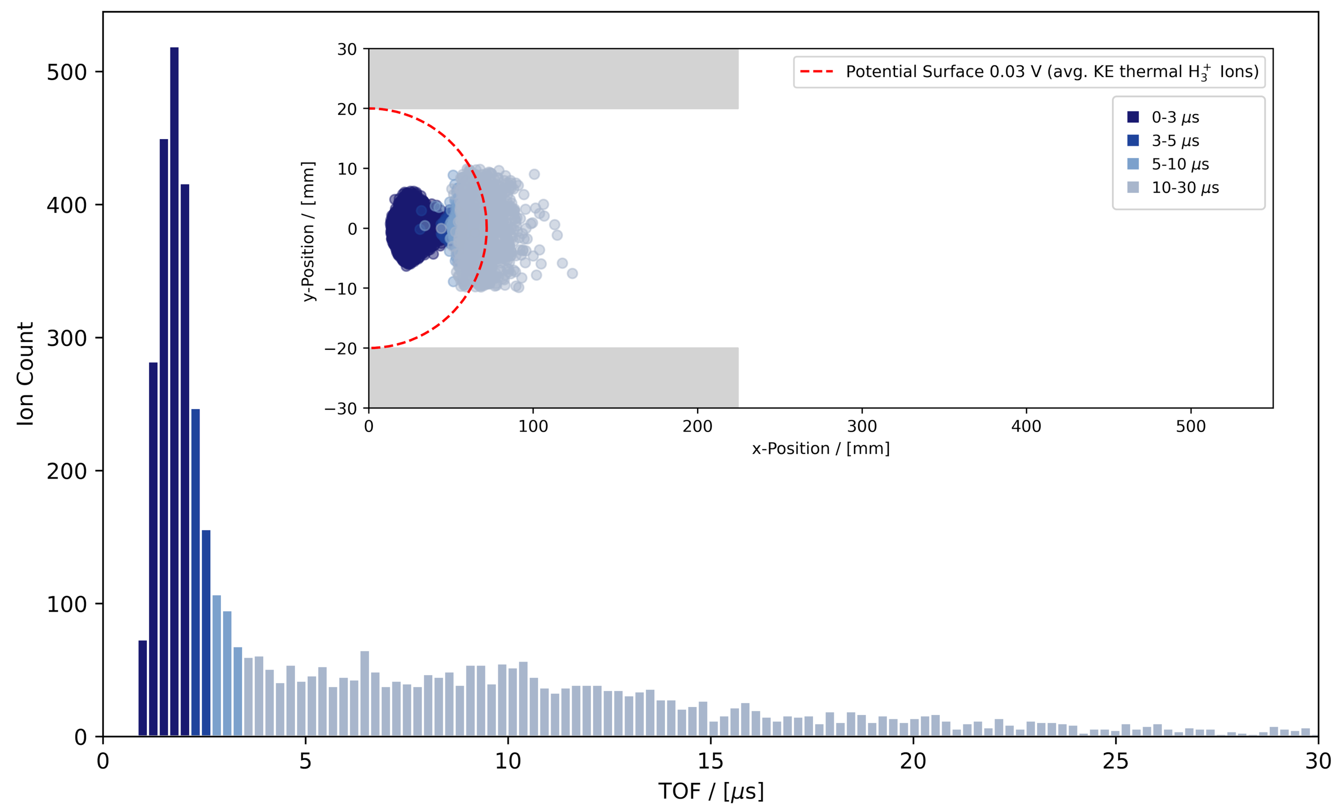

Figure 5: Breakdown of bulk sampling regions by time-of-flight (TOF)

- Temporal **and** spatial sampling possible
- Examination of anisotropic, chemically diverse plasmas
- Relevance for photo-induced plasmas

Different ion starting regions can be separated and identified by time of flight.

Outlook

Since the preliminary results are promising, further investigation is warranted. An extension of the pressure study as well as simulations for different m/z ratios (and corresponding collision cross sections) are planned. Moreover, a higher resolution may be achieved by upscaling the total number of simulated ions and consolidating the starting locations towards the interesting region (cf. Fig. 1 and 5). Simulations at higher ion densities in PICLas might enable the evaluation of space charge effects.

References

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[2] Fasoulas, S., Munz, C.D., Pfeiffer, M., Beyer, J., Binder, T., Copplestone, S., Mirza, A., Nizenkov, P., Ortwein, P. & Reschke, W. (2019). *Physics of Fluids*, *31*(7), 072006.

[3] Geuzaine, C. & Remacle., J.-F. (2009). Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities. *Int. J. Num. Meth. Engng.*, *79*(11), 1309-1331.

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