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

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Introduction

In virtually all ion sampling scenarios, a pressure gradient between vacuum recipient and a transfer stage / the mass spectrometer needs to be maintained. The interface is then often realized as an electrostatic guide through a narrow, gas-flow restricting aperture. In this work, the sampling efficiency of a lens system with a smallest orifice radius of 0.25 mm is examined, which serves as the separator between a plasma region and the transfer system of a time-of-flight mass spectrometer (TOF-MS). For the ions located directly in front of the restrictor, a strong dependence of the transmission chance on initial position is expected. The purpose of this study is to quantify the sampling efficiency of the aforementioned setup with respect to background gas pressure and initial ion kinetic energy.

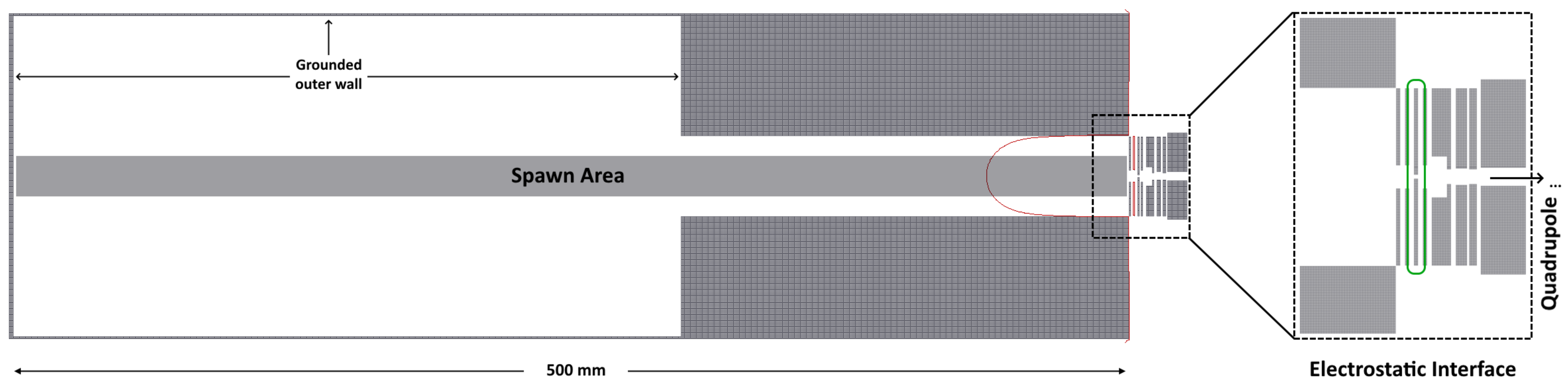

Figure 1: Simulation domain with 0.03 V equipotential line (red, referring to thermalized ions) and electrostatic interface (with dummy quadrupole)

Methods

Simulations were carried out for variable pressure and ion kinetic energy. The sampling efficiency was visualized statistically at different starting positions.

H_3^+ ion trajectories were calculated with the SIMION program package[1]. A hard-sphere collision model was employed in order to test the pressure dependence of the ion movement.

Due to time constraints, thus far no comparative study with the particle in cell and DSMC based plasma simulation software PICLas[2] was conducted. This is planned for the near future; for further info please refer to the Outlook section.

Results

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

Unlike pressure, the simulations show a strong dependence on initial ion kinetic energy. The 2D-histogram in **Figure 2a** reveals a distinct shape for the bulk region of sampled ions which is thought to be the projection of the geometric and electrostatic configuration of the interface with regard to transmission. The shape becomes increasingly blurred with higher starting energies, which is in accordance with the theory that the initial ion phase space suitable for transmission is mainly governed by the electrostatic landscape created by the lens stack.

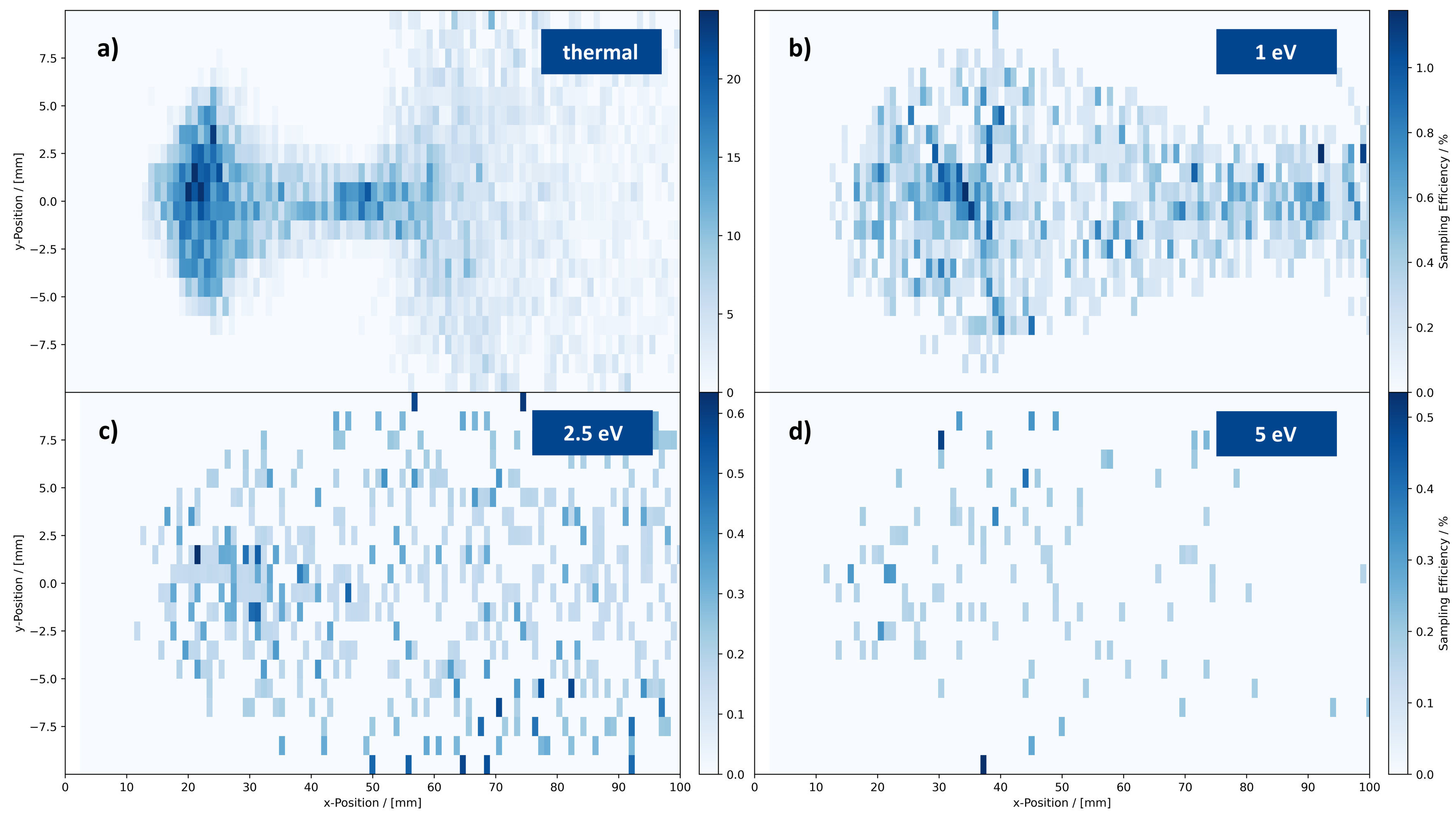

Figure 2: Transmission efficiencies for different starting velocity distributions

The depiction in **Figure 3** highlights the various ion travel times from different "sampling hotspots", which can be resolved by a mass spectrometer with sufficient temporal resolution. Regarding such a measurement, the simulations provide valuable insights regarding the temporal profile of ionic species sampled from an anisotropic, chemically diverse space, which is especially interesting for photo-induced plasmas.

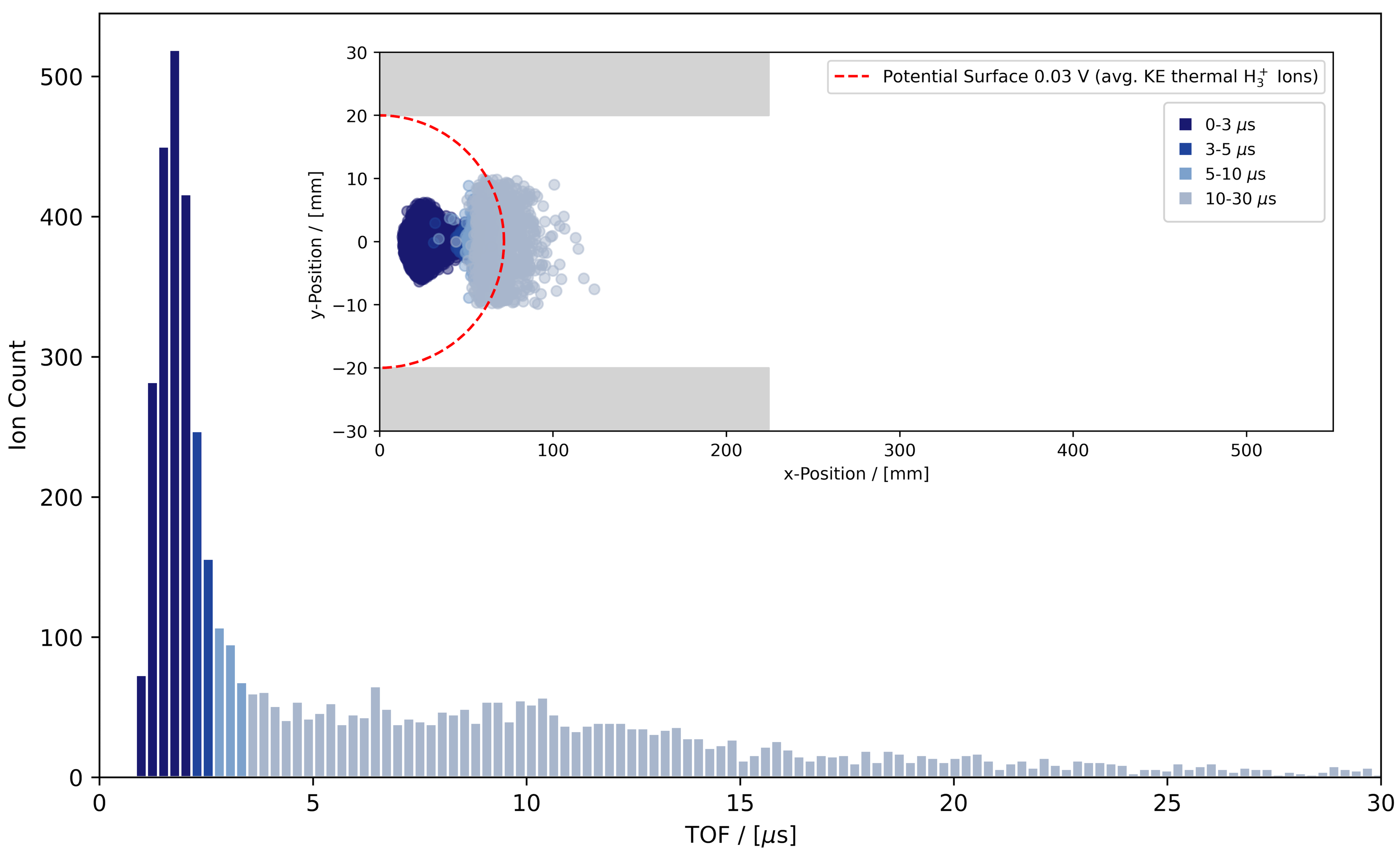

Figure 3: Breakdown of bulk sampling regions by time-of-flight (TOF)

Outlook

Since the preliminary results are promising, further investigations are planned. An extension of the pressure study as well as simulations for different m/z ratios (and corresponding collision cross sections) are scheduled. 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 3). Unfortunately, no calculations with PICLas were included thus far. Hopefully, a comprehensive comparison as well as additional results will be presented at the 2024 ASMS conference in Anaheim.

References

[1] Dahl, D.A. (2000). *Int. J. Mass Spectrom.*, *200*(3), 3-25. [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.