An efficient ion funnel operating at 100 mbar background pressure

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Introduction

Ion funnels are known to work well at pressures below 30 mbar [1] (cf. Fig. 1). In this work, a 5 mbar ion funnel has been designed based on simulations. Sensitive parameters are scaled for an operation at pressures of 100 mbar and higher. As a result a highly sensitive CIMS instrument is designed, which allows to drive the analyte ion chemistry at 100 mbar within the first ion funnel. Additional simulations of the ion funnel at 100 mbar, including the fluid dynamics, electrostatic fields and the resulting ion trajectories, are presented. The results of the calculation and the simulation are validated by experimental data, e. g. the transmission of the ion funnel at 100 mbar.

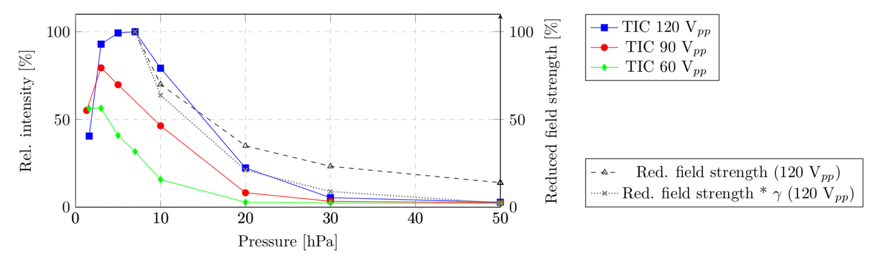

Figure 1 The total ion count measured at different pressures and voltage amplitudes (at 1.8 MHz) applied to a funnel with an electrode distance of 0.5 mm (Stage 2, Fig 2). The second vertical axis shows the reduced field strength.

Methods

A Tofwerk "HTOF" (Thun, CH) time of flight analyzer was fitted with a custom high transmission differential pumping stage consisting of an ion transfer capillary sampling at AP, followed by two ion funnels and a transfer quadrupole, as shown in figure 2. The background pressure of the ion funnels is controlled by butterfly valves. Critical parameters, e.g. the flow through the ion funnel are controlled for optimal transmission. Ions are generated by a dielectric barrier discharge ion source.

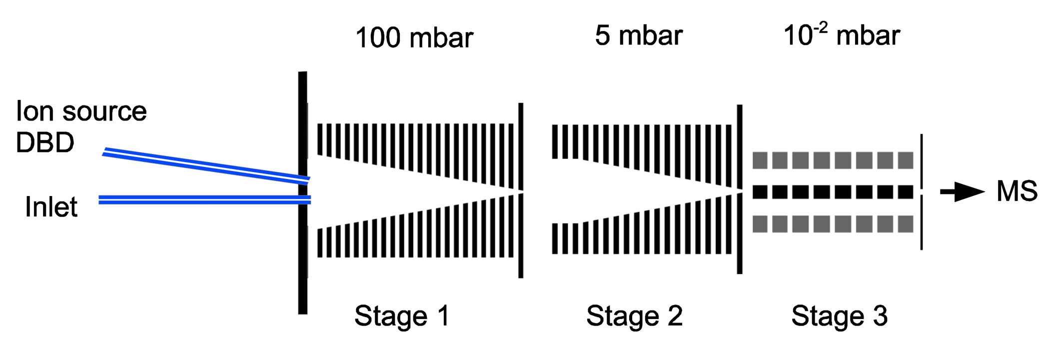

Figure 2 A schematic drawing of the CIMS transfer stage.

Construction

The ion funnel consists of 120 electrodes, made of 0.25 mm thick stainless steel using a distance of 0.25 mm between the electrodes. The electrodes are gold coated (2 µm) against reactive chemicals, which also enables soldering of the electrodes to a printed circuit board. The inner diameter of the electrodes linearly decreases from 20 mm to 2 mm. The overlapping area of the electrodes with opposite RF signals is minimized in order to reduce the total capacitance of the ion funnel (cf. Fig. 3). Six fixtures arranged hexagonally are used for the electrodes, three for each of the phase shifted RF-signals. Only every second electrode is mounted on each fixture.

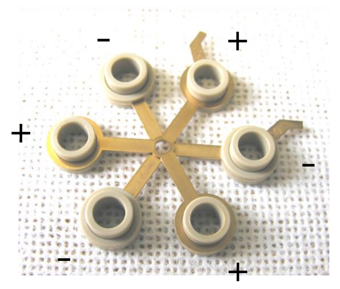

Figure 3 The two smallest electrodes of the ion funnel with the PEEK spacers.

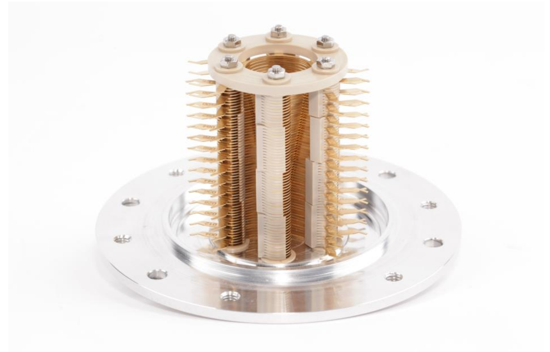

Figure 4 A photo of the 100 mbar ion funnel before the printed circuit boards are attached.

Fluiddynamic effects

The gas velocity is a critical parameter for the transmission of the ion funnel. The ion funnel is driven with 120 V_{pp} at 5 mbar. The pressure is kept constant by a butterfly valve and an additional flow of nitrogen is added concentrically to the capillary. The flow through the DBD was 1 slm. As a result all parameters were kept constant but the flow through the ion funnel was increased. Fig. 5 shows that an increased flow of 60 % decreases the ion transmission by approximately 20 %. The fluid dynamic simulation has shown that the flow velocity in the ion funnel is quite high (Fig. 6). The required electrostatic field is directly proportional to the flow velocity.

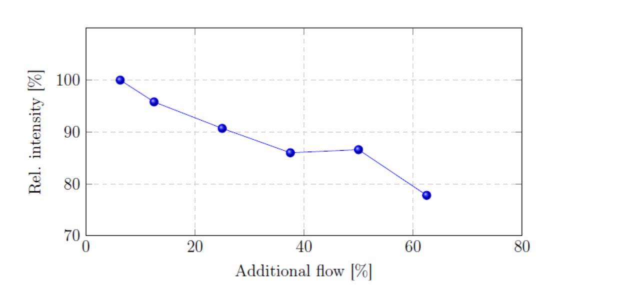

Figure 5 The total ion count measured with an additional gas flow added concentrically to the flow of the DBD (1 slm) feeding the 5 mbar ion funnel.

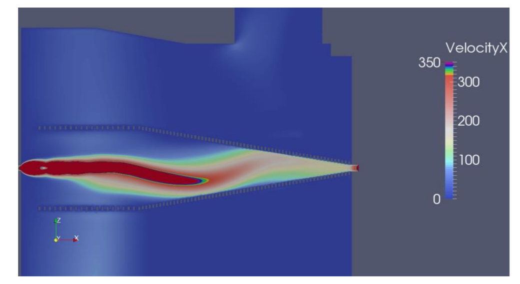

Figure 6 A cut through the simulated flow field of the 5 mbar ion funnel with the velocity in x-direction in m/s.

Scaling of ion funnel parameters

The maximum effective potential U_{eff} characterizes the potential that affects the ions and is used to compare different operation modes of the ion funnel. Here, ω is the angular frequency, V_{RF} is the voltage amplitude of the RF-field, m is the molecular mass of the ion, q is the charge of the ion, and $\delta = d/\pi$, where d is the distance between the electrodes. Tolmachev et al. suggested an additional term γ [4]. It specifies the effectiveness of the RF-field suppression near the high pressure limit. This results in the effective potential U_{eff}, which takes account of the ion mass, the electrode distance and the pressure dependence.

$$\gamma = \frac{\omega^2 \tau^2}{1 + \omega^2 \tau^2} \tag{1}$$

$$U_{eff} = \gamma \frac{q V_{RF}^2}{4\, m\, \omega^2 \delta^2} \tag{2}$$

$$\tau = \frac{3(m+M)}{4\, m} t_{col} \tag{3}$$

Simulation of the 100 mbar ion funnel

Fluiddynamic calculations have been performed with the commercial software package Ansys CFX 14 (Ansys, Inc., USA). The flow through the ion funnel is approximately 5 slm. The fluid dynamic data are used in the SIMION/SDS simulation, which includes the effects of the reduced field strength and the collision frequency. The simulation results show that the ion funnel works properly at 100 mbar background pressure. Each of the simulation runs (Fig. 8-10) took about 14 days on a standard PC using the final results of the fluid dynamic simulation. Each time steps need to be scaled to the driving frequency of the ion funnel. For the simulation a frequency of 10 MHz is used, therefore the effective potential is reduced by a factor of 0.6 (γ) mainly caused by diffusion.

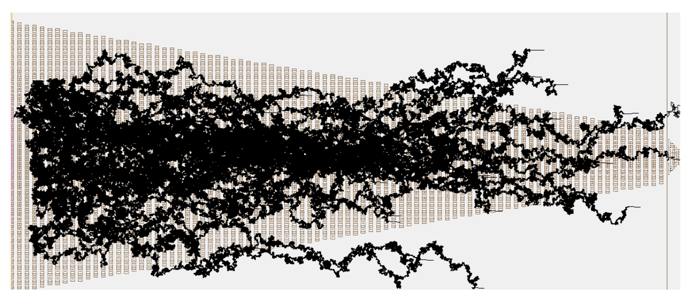

Figure 8 A cut through the Simion SDS ion trajectory simulations of the ion funnel at 100 hPa driven with 200 Vpp and 10 MHz. In black the ion trajectories of 40 ions with mass 100 are shown.

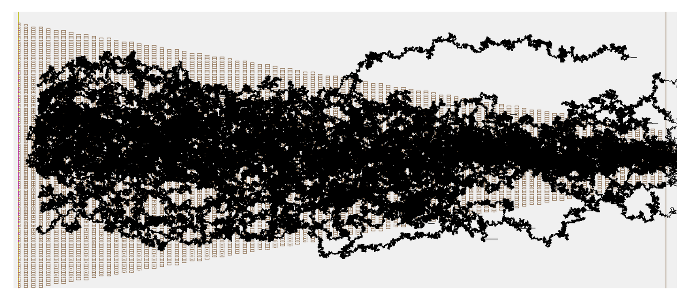

Figure 9 As figure 8 but for 300 Vpp.

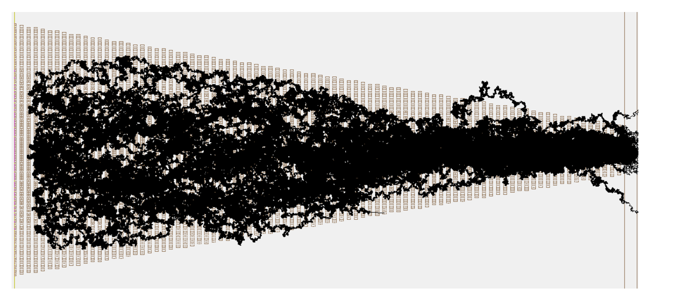

Figure 10 As figure 8 but for 400 Vpp.

Conclusions: Limits of ion funnels

The results obtained for the 100 hPa ion funnel (300 V_{pp} at 10 MHz, 50 % ion transmission, m/z = 100) can be scaled to other pressures and electrode distances. The following assumptions are made: The flow velocity is constant. The frequency increases linearly with pressure keeping the damping of the electrostatic field by diffusion constant. The breakdown voltages are calculated using the equations of Burm [2]. Comparing the breakdown voltage and the required voltage amplitude shows that the constructed 100 mbar ion funnel with 0.25 mm electrode distance is operating close to the breakdown limit. If the electrode distance can be reduced to approximately 25 µm, e.g. using a planar ion funnel [3] even an operation at atmospheric pressure becomes possible (cf. Fig. 7). However, the estimated driving power is in the order of 1 kW.

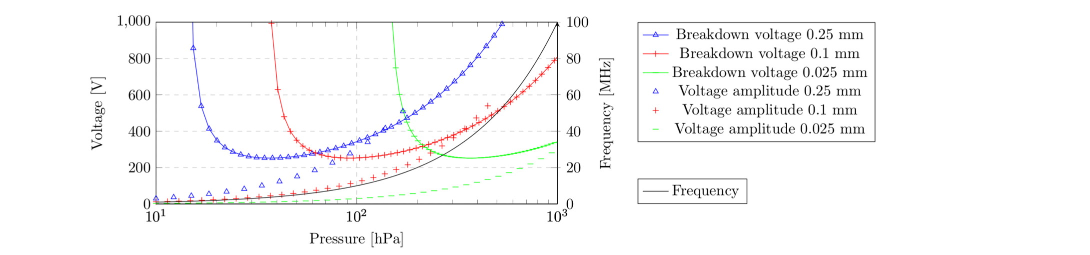

Figure 7 The results of the 100 mbar ion funnel scaled to a broad pressure range using equations 1 and 2. Additionally the breakdown voltages for each plotted electrode distance is given.

Transmission measurements

The transmission of the ion funnel operated at 100 mbar has been calculated using the ion currents measured upstream the ion funnel and after the nozzle downstream of the ion funnel by means of a Faraday cup and a custom electrometer. A transmission of 30 % has been measured operating the ion funnel at 100 mbar, 240 V_{pp} and, 10 MHz, which agrees well with the simulation.

Literature

[1] Page, J. S., Kelly, R. T., Tang, K. & Smith, R. D. Ionization and transmission efficiency in an electrospray ionization–mass spectrometry interface. *Journal of the American Society for Mass Spectrometry* 18, 1582–1590 (2007).

[2] Burm, K. T. A. L. Calculation of the Townsend Discharge Coefficients and the Paschen Curve Coefficients. *Contributions to Plasma Physics* 47, 177–182, (2007).

[3] Van Amerom, F. H. W., Chaudhary, A. & Short, T. R. *Planar ion funnel* US Patent 20,130,120,894. (2013).

[4] Tolmachev, A. V., Chernushevich, I. V., Dodonov, A. F. & Standing, K.G. A collisional focusing ion guide for coupling an atmospheric pressure ion source to a mass spectrometer. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 124, 112–119 (1997).

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