Ion-atom interactions in a gas jet - coupling of a gas catcher to a linear RFQ cooler

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Several existent add-on models allow the inclusion of a gas-ion interaction in SIMION. A comparison is made between the performance and applicability of hard-sphere (HS1) model, Statistical Diffusion Simulation (SDS) model, and viscous drag model. This comparison includes a definition of an atomic gas jet from a nozzle separating a high pressure region ($P_0 \approx$ few hundred mbar) and a constant low background pressure region. The gas jet is defined by several input parameters (temperature, pressure, velocity) which vary in space and depend on P_0, T_0 and d_0 (Fig. 1). Depending on their coordinates the ions of interest are interacting with the gas jet and/or the background gas with different interaction cross sections. The gas atom-ion interactions together with applied DC potentials on extraction electrodes guide the ions into a Radio Frequency Quadrupole cooler where the ions are confined by the oscillating electric fields and their subsequent interaction with the background gas leads to thermalization (cooling).

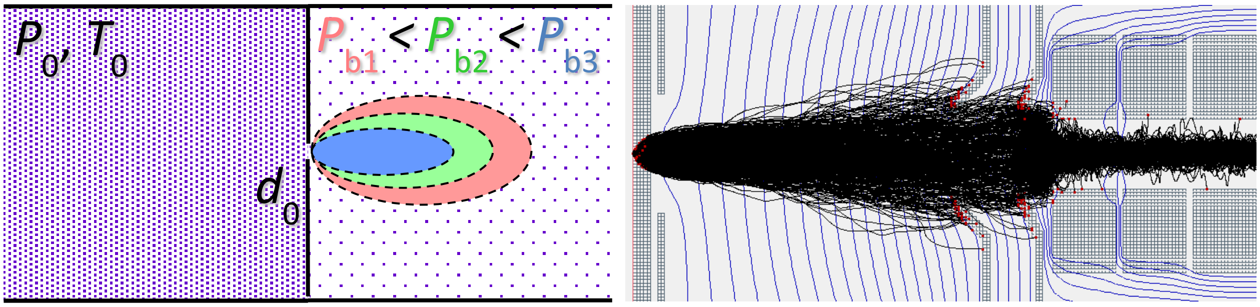

Figure 1. The left side shows two gas volumes at different gas pressures separated by a simple aperture nozzle. The pressure difference is maintained by differential pumping forming a free expansion gas jet the properties of which depend on P_0, T_0 and d_0 but also on the background pressure P_b (higher background pressures limit the size of the jet and the effects of the jet on the ions). The right side shows trajectories of ions at the low pressure region interacting with atoms from the jet and the background gas. This simulation was used in order to optimize design parameters for the highest loading efficiency into the RFQ cooler.

The initial geometry of the nozzle, extraction electrodes and the S-shaped RFQ cooler are shown in Figure 2. The loading of ions into the RFQ structure is done by applying DC potentials whereas for the radial confinement inside the RFQ also oscillating RF potentials are applied on the RFQ electrodes.

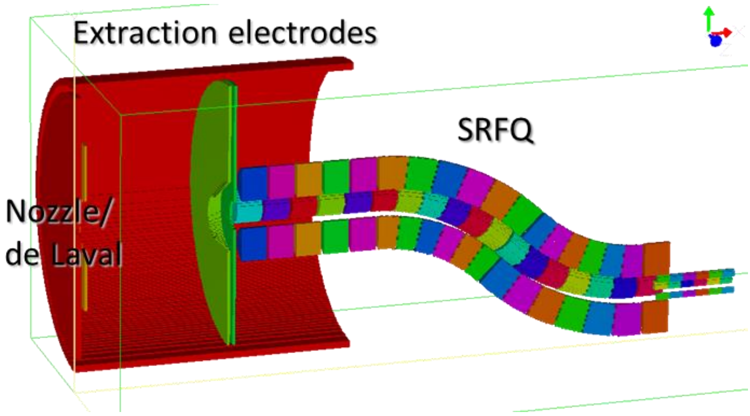

Figure 2. The initial geometry of the electrodes used in the SIMION simulation.

The viscous drag model is based on measured ion mobilities and in its original form it does not allow inclusion of ion-atom interactions. For this reason only SDS and HS1 models were used in the simulations in the vicinity of the gas jet region. The documentation of SDS indicates that this model should not be used at low pressures due to the statistical approach that it utilizes for a faster calculation compared to the HS1 model. The low pressure limit of SDS was determined by the simulations at different background pressures after loading into the RFQ. Figure 3 shows an example at 0.01 mbar of Ar where the statistical approach of SDS fails due to the inability to confine the ions in the RFQ volume at confinement settings.

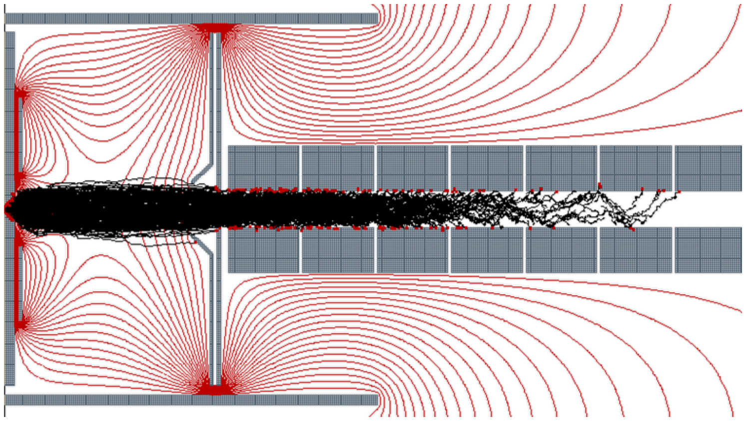

Figure 3. Example of confinement loss in the RFQ using SDS at 0.01 mbar.

The pressure region at which the SDS starts failing was found to correspond to a mean free path of interaction being in the order of the distance between the electrodes (~ 10 mm). A comparison with the HS1 model shows significant disagreements in loading and transmission efficiencies already at pressures below 0.1 mbar. The latter was the reason to discontinue the use of SDS in our simulations since the range of expected background pressures overlap with the pressures at which unstable SDS results were observed. HS1 was used for the entire range of pressures up to 0.5 mbar although the calculation time required for one simulation at the highest pressure was more than 20 hours for 1000 particles.

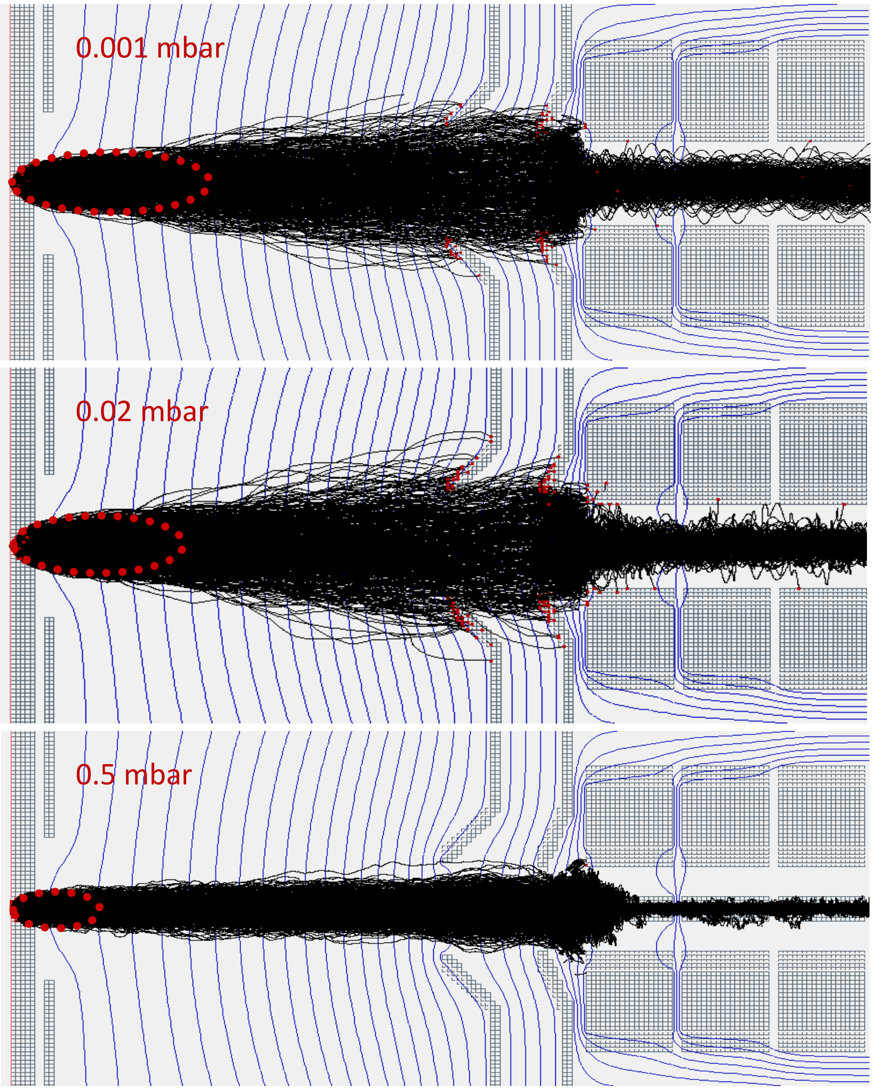

Figure 4. Example of loading into the RFQ at different background gas pressures using HS1 model.

The gas jet definition as well as other gas pressure, temperature and velocities can be defined in two ways in SIMION. The first approach can be used if these parameters can be obtained by equations depending on known parameters as in our case where we used the approach described in [1]. The other approach is to use an external simulation (e.g. COMSOL, ANSYS, etc.) and obtain pressure, temperature, and velocities maps into files as explained in the SDS documentation but not limited to the use of SDS.

Figure 4 contains trajectory plots for three different background pressures (0.001 mbar, 0.02 mbar, and 0.5 mbar) using HS1 model. At low pressures the gas jet directs the ions towards the entrance electrodes where they are guided by DC fields. The size of the gas jet is becoming limited at higher background pressures and the push effect on the ions is reduced with increasing background pressure. With a further increase of the pressure the ions are thermalized well before the entrance electrodes and after they are guided by diffusion and DC fields towards the entrance of the RFQ cooler. This interplay of effects can explain the observed drop of loading efficiency (increased losses by hitting the electrodes) at intermediate pressures (Red squares in Fig. 5). The observation of the sites of losses allowed us to optimize the design of the entrance electrodes and the RF structure in order to minimize losses (Blue/grey triangles in Fig. 5).

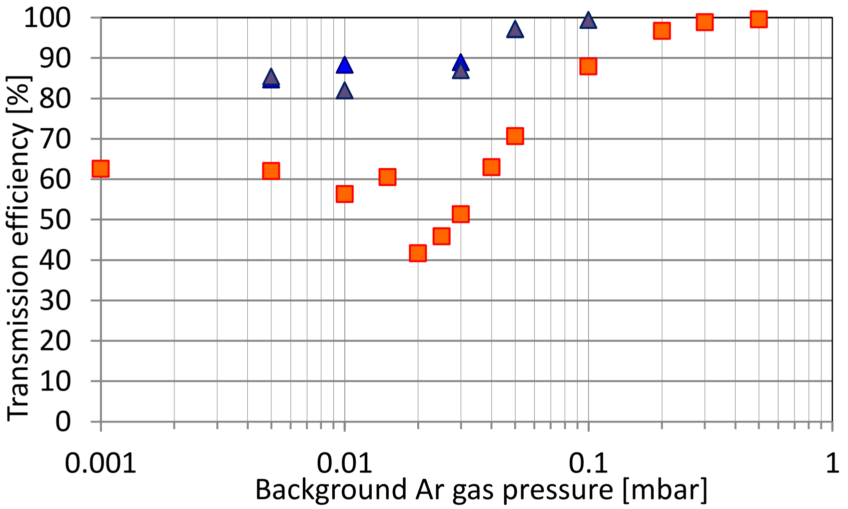

Figure 5. Efficiencies at different pressures before (squares) and after (triangles) design optimization.

The variation of results after the design optimization (the blue and grey triangles in Fig. 5) is due to different DC settings in the two cases. The final optimized design of the system is shown in Figure 6.

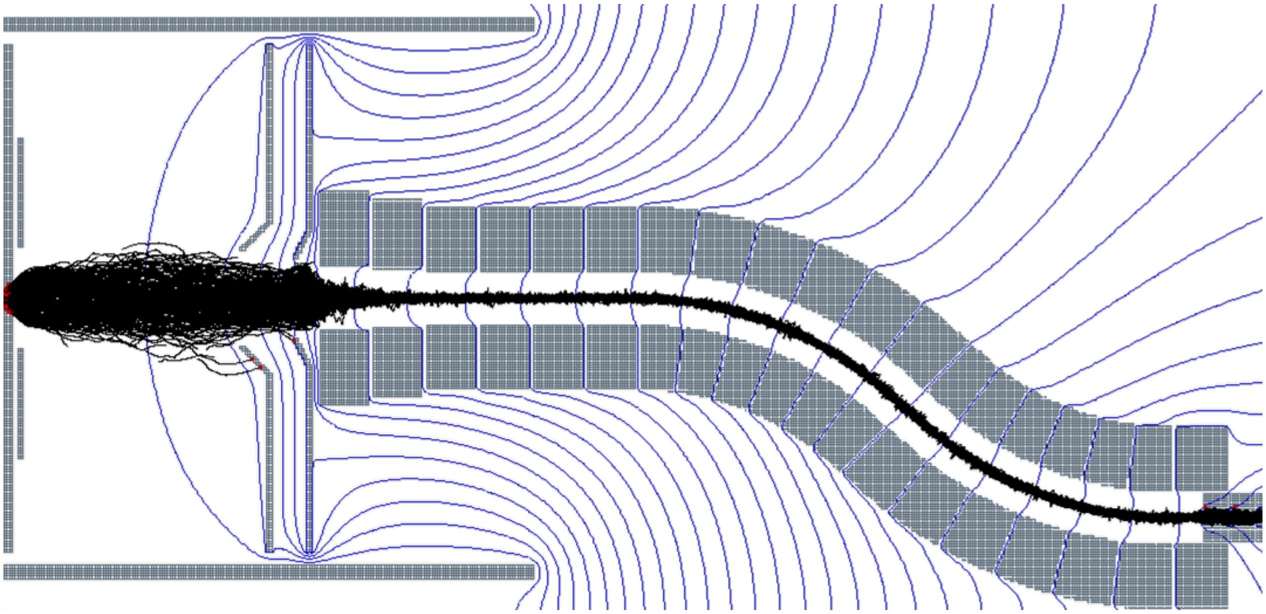

Figure 6. Final design of the extraction electrodes and entrance RFQ electrodes after optimization.

An important comparison between HS1 model and viscous drag model was made in order to define possible miscalculation of the necessary gas pressure by HS1 model (as indicated in the HS1 documentation on the website of SIMION). The viscous drag models is based on measured ion mobilities therefore results from gas cooling in the RFQ can be used as a reference for comparison with the cooling achieved in the HS1 model. Figure 7 shows an example of the two simulations at 0.13 mbar of Argon buffer gas using the same input distribution of ions before the entrance of the RFQ cooler. The results suggest that lower pressures than the ones estimated by the hard-sphere model may be sufficient for the purpose of cooling (kinetic energy and transverse emittance reduction). The comparison was made for Rb^+ ions in Argon gas due to the known (measured) ion mobility [2] but a similar result is expected for other ion-gas combinations due to general underestimation of long-distance ion-atom interactions by the HS1 model at ion kinetic energies below several eV [3].

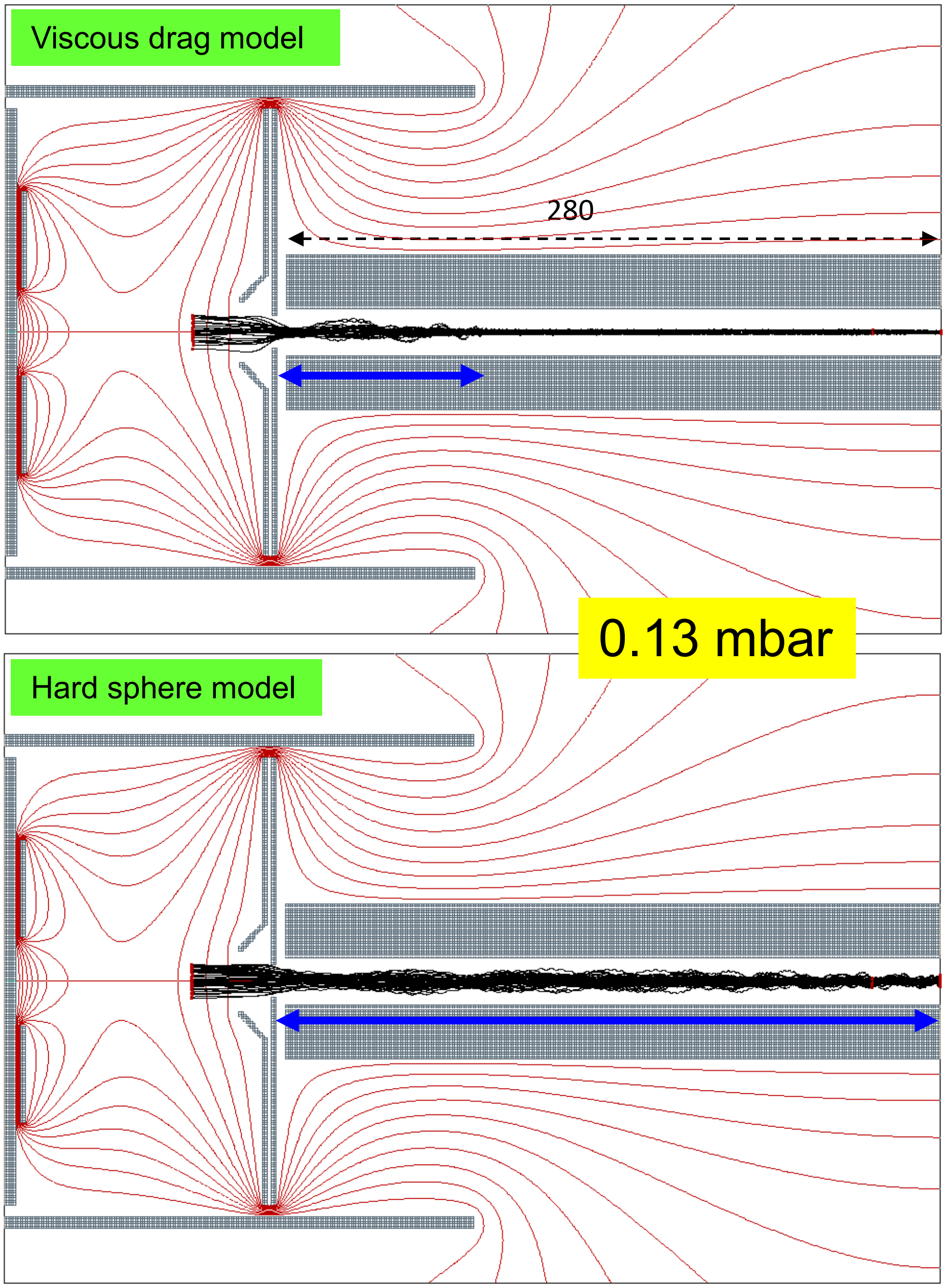

Figure 7. Comparison of cooling by viscous drag and HS1 models. The results show that for the same buffer gas pressure of Argon (0.13 mbar) the same amplitude damping is achieved much faster in the viscous drag model compared to the HS1 model.

References:

[1] Yu. Kudryavtsev, *et al.,* Nucl. Instrum. Meth. B 297 (2013) 7

[2] H.W. Ellis, *et al.,* At. Data Nucl. Data Tables 17 (1976) , 22 (1978) , 31 (1984)

[3] M.D. Lunney, R.B. Moore, Int. J. Mass Spectrom. 190/191 (1999) 153

Other general notes and tips on using SIMION

1. In certain cases it is convenient to combine different add-on scripts in SIMION without modifying the original files. An easy way to do this is to combine .lua and .prg files. SIMION will work correctly as long as the two different scripts do not modify simultaneously the same SIMION internal parameter, e.g. time step size.

2. « surface=fractional » can increase significantly the precision of the simulation without the necessity to increase the number of grid units/mm.

   e.g.: PA_define(1200,400,400,p,n,surface=fractional)

3. For simulations using very large accelerations a large quality factor T_qual should by used (T_qual_max. = 500) but this may slow down significantly the simulation. ΔKE can be accessed in the data recording menu for choosing an optimal value for T_qual.

4. A very simple and useful 2D CAD import can be done by using SL tools of SIMION. A scan of a geometry and colouring of different electrodes by different colours can be save as a .bmp file and converted to .pa files (Bitmap -> PA)

   (see: http://simion.com/info/sltoolstut.html)

5. Particles can pass through very thin electrodes in SIMION. A way to stop this is to use thicker electrodes (>1 g.u.)