TECHNICAL NOTE

Liquid Chromatography/
Mass Spectrometry

Ion Transmission Through a Quadrupole Ion Guide Under the Combined Influence of Viscous Flow and RF Electric Fields

Most mass spectrometers sample ions from atmospheric pressure. As such, it is of interest to maintain the ion flux while removing surrounding gas as the ion flux progresses from the atmospheric ion source to often below 10^{-5} torr. With modern mass spectrometers, there are series of intermediate pressure regions. The radiofrequency (RF) quadrupole guide is commonly used in mass spectrometry for the transport of ions produced at atmospheric pressure into a mass analyzer operating under high vacuum. The effective potential produced by RF moves ions to the centerline therefore significantly reducing ion losses, whereas the gas flow transports them downstream. Figure 1 shows that gas collisions suppress ion oscillation and that gas flow assists in overcoming the reflecting fringe fields in the entrance. Here we determine through numerical simulations the physical conditions necessary to obtaining maximum ion transmission of the first ion guide maintained at approximately 1.5 torr. In this first ion guide the gas flow drag and electric field forces can be made to have a comparable level of influence upon ion motion: their combination can be optimized for ion transmission.

The first ion guide region is shown in Figure 1, with arrows illustrating the flow of gas and ions propagating left to right from a 5 mm diameter aperture (entrance lens not shown) through the four cylindrical electrodes. Some of this gas flow enters the aperture (3 mm diameter) of an exit lens to a lower pressure chamber, with the bulk of the flow being removed by a roughing pump.

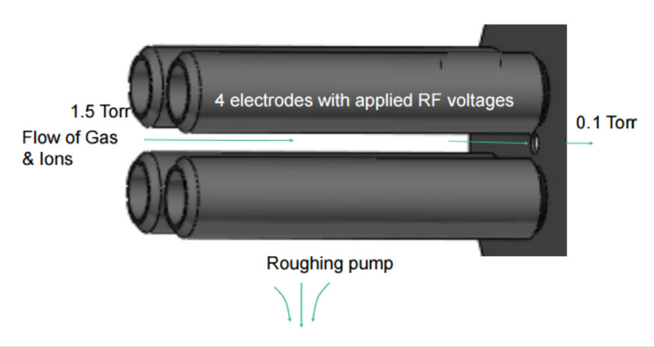

Figure 1. First ion guide region.

Numerical study of the ion motion through the ion guide is provided. The simulation data is obtained using commercially available numerical computational codes: the calculation fluid dynamics (CFD) program is ANSYS FLUENT[2] (6.2.12 version) and the ion optic program is SIMION[3] (8.1 version). First, the flow field is calculated using the Spalart – Allmaras turbulent model. Flow calculations are performed using finite – volume analysis with second order discretization. Second, these gas flow field velocity characteristics are imported into SIMION. The simulations in SIMION are based on the Stokes law model[4]. Turbulent diffusion is taken into account using approximate empirical theory, described in reference 5. The new modification of Statistical Diffusion Simulation (SDS) collision model, which incorporates turbulent diffusion estimation, is developed in private communication with SIMION developers[6].

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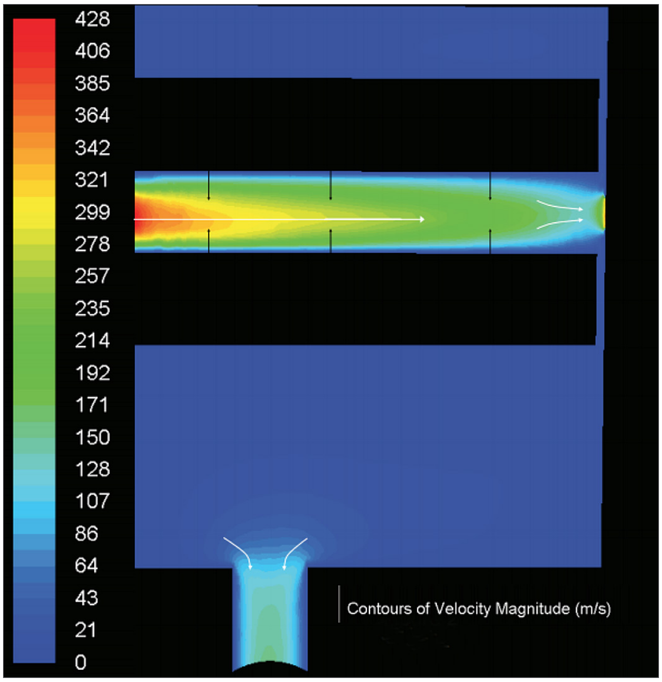

Figure 2. Contours of velocity magnitude.

Figure 2 shows contours of velocity magnitude (ANSYS FLUENT calculations) flow, and effective electrical field vectors (white and black arrows, respectively). The gas flow with the ions propagates into the center of the quadrupolar rod array, then it bifurcates with first part going into second chamber through the aperture, and the second part flowing principally between the four gaps between the rods. Ideally, the ions don't go between the rods with second part of flow, because they are contained by the effective RF electrical field.

Results

Ion Trajectories

Each simulation run uses a set of 100 ions randomly distributed across the surface of the 5 mm diameter entrance lens. Ion charge is – e, mass is 59 u.

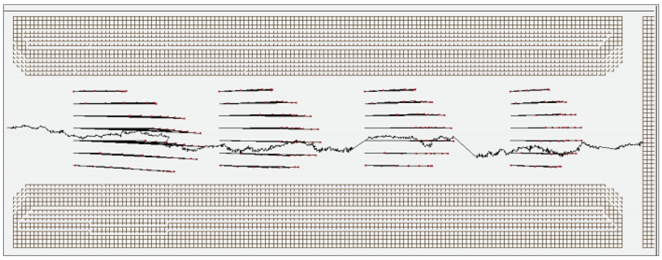

Figure 3. Example of a single ion trajectory between the quadrupole rods, with straight lines representing mean gas flow velocity field: the trajectory ends at the exit lens. Ion q-value is 0.1006. We see that the ions roughly follow the mean flow. Small oscillations relate to molecular diffusion, whereas large displacements relate to turbulence.

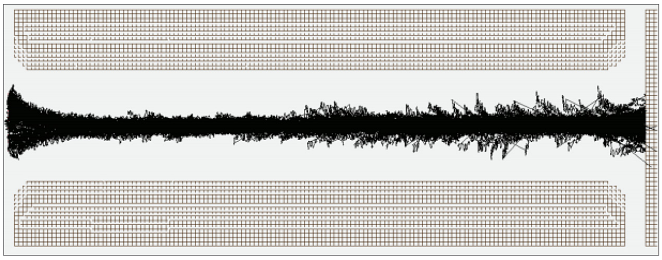

Figure 4. Ion q-value is 0.402 set of 100 ions (coulomb repulsion included). This is a stable condition for quadrupolar containment (first stability region of a linear quadrupole,[7]). After turbulent displacements, the focusing effective field returns ions to the quadrupole axis.

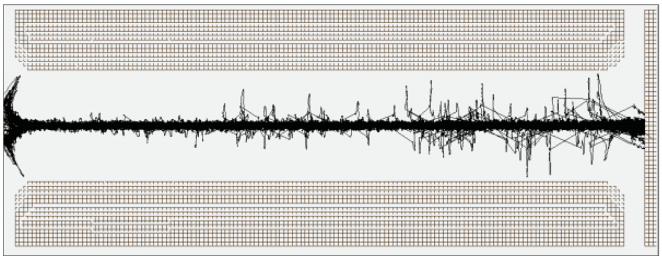

Figure 5. Ion q-value is 1.00 set of 100 ions (coulomb repulsion included). Although this larger effective electric field is an unstable condition, the ion trajectories are observed to be more confined to the axis. Whereas 2/3 of the ions go through the exit aperture, 1/3 of the ions are lost principally because they hit the rods or entrance lens due to entrance fringe fields. As in Fig. 4, the focusing effective electrical field also returns the ions to the centerline region after turbulent effects.

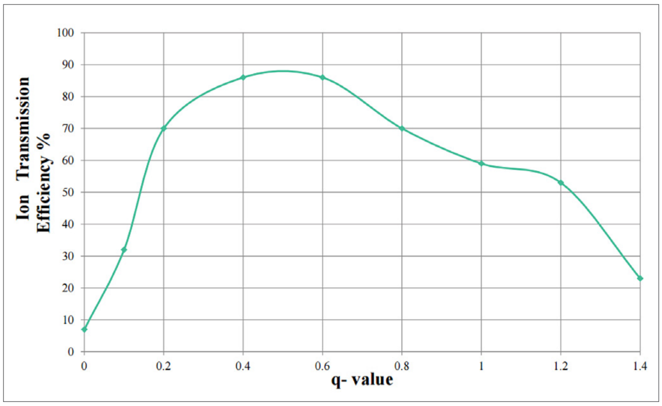

Figure 6. Ion transmission efficiency vs ion q-value - numerical simulation from 9 q-values. The drift of ions to the axis increases with q-value, and the inherent instability due to ions absorbing energy from the field is prevented by ion-gas collisions.

Conclusion

Initial simulations of ion motion in an RF ion guide with turbulent flow at 1.5 torr show that ion transmission is critically dependent upon ion q-value: moreover the transmission efficiency from entrance to exit can be nearly 90% at the appropriate q-value.

Even in regions where the ion is traditionally unstable ($q > 0.9$), the ion transmission is about 70%.

References

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