Ion guide for improved atmosphere to mass spectrometer vacuum ion transfer

Authors: Hassan Javaheri and Bradley B. Schneider

ABSTRACT

Various approaches for transmitting ions from atmosphere to the deep vacuum required for mass analysis have been developed with the goal to increase the ion to gas ratio while maintaining high ion transmission efficiency. Since the vast majority of ion losses occurs in the atmospheric pressure ion source, an effective way to improve sampling of those ions is to increase the atmosphere to vacuum aperture diameter. However, as the aperture diameter is increased, the resulting intense free jet gas expansion and subsequent gas beam can scatter ions in the first vacuum region. The interface described here provides an optimized flow field to the second vacuum stage, with a unique geometry to counter the ion losses from scattering collisions with the gas. Two additional differentially pumped quadrupole ion guides are used to further improve the ion to gas ratio, resulting in an ion transfer efficiency improvement of 5−6 × over a two-stage differentially pumped interface with quadrupole ion guides. The interface also demonstrates efficient declustering and fragmentation capabilities beneficial for reducing background chemical noise.

INTRODUCTION

Ionization at atmospheric pressure is a highly efficient process using either electrospray or atmospheric pressure chemical ionization. Sampling efficiency refers to the percentage of molecules entering the ion source that are converted into ions and successfully transported into the vacuum system. The greatest losses occur as a result of the low transfer efficiency from atmosphere to vacuum, because ions are scattered by gas flows in the ion source. An effective way to improve the transfer efficiency is to sample more gas using larger atmosphere to vacuum apertures. A variety of different approaches have evolved over the years to increase the gas loads and, therefore, ion transfer into the vacuum system, followed by means of increasing the ion to gas ratio prior to the ion beam entering the mass analyzer, including the use of quadrupole rods, ion funnels, and ring guides. As gas flows are increased, the challenge is to maintain control over the trajectory of the ion beam in the initial stages where collisions with the background gas scatter the ions in the shock waves that develop when sampling ions from gas beams with Mach Velocities.

MATERIALS AND METHODS

A novel high gas throughput interface configuration was designed (Figure 1) and the analytical performance was compared to a standard triple quadrupole instrument (SCIEX Triple Quad 6500+ system). The novel inlet included an additional differentially pumped vacuum stage with a dodecapole ion guide, installed prior to the D Jet ion guide region. The inlet orifice was opened to boost the gas throughput from approximately 4 L/min to about 16 L/min. The vacuum pump speed was increased to handle the high gas loads from the larger inlet orifice.

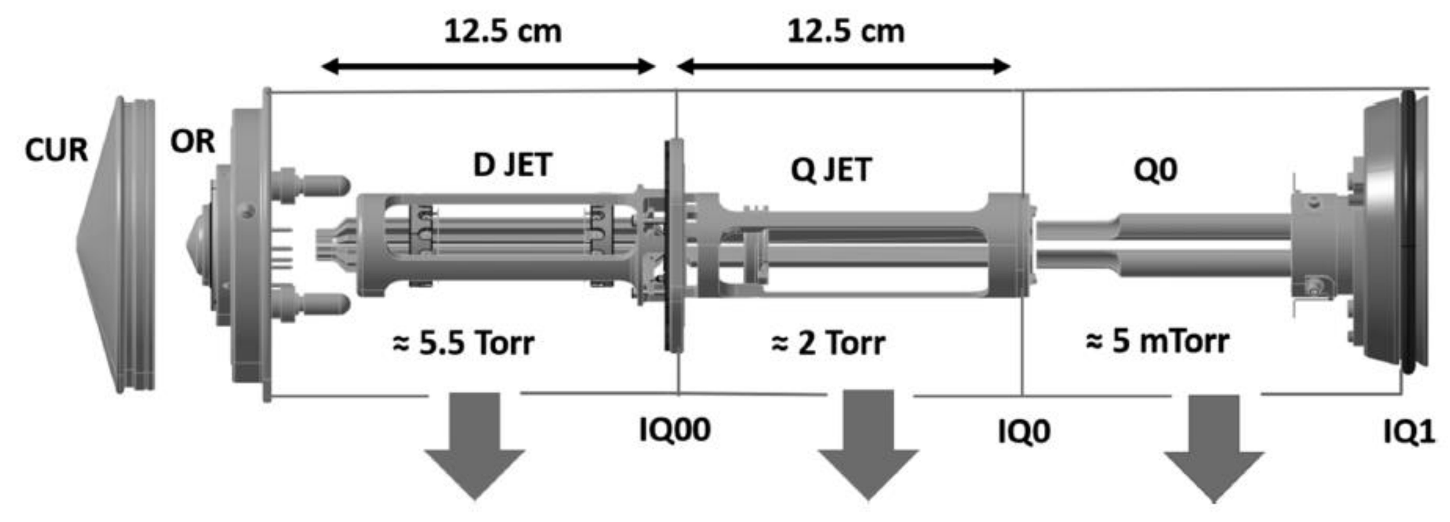

Figure 1. Novel high gas throughput interface configuration.

LC-MS experiments were conducted using a Shimadzu LC20ADXR LC system and Millipore Ascentis Express C18 column to compare the analytical performance of the novel D Jet ion guide inlet system to the standard QJet ion guide inlet system. The instrument was the same from the Q0 ion guide to the detector for the two interface configurations. Sensitivity improvements were evaluated by comparing the absolute signal intensities for on-column injections of a large number of compounds with a range of precursor and product ion masses, including both ionization polarities.

CFD Modeling

Computational fluid dynamics (CFD) modeling was conducted to improve our understanding of the gas flow characteristics through the D Jet ion guide. CFD simulations were performed using the CFD++ commercial software suite (Metacomp Technologies). Temperature and pressure measurements were taken on the breadboard at various locations on and around the inlet orifice, D Jet ion guide chamber, and QJet ion guide chamber, and these values were used in the CFD calculations. Figure 2 shows the calculated Mach number for the gas flow through the first vacuum stage (D Jet ion guide structure shown in white). The gas flow accelerates to a maximum Mach number of approximately 6.73 and forms a Mach disk near the front of the dodecapole rods. The inlet acceptance diameter of the D Jet ion guide was similar to the diameter of the barrel shock for the gas flow through the 1.5 mm orifice, ensuring that the bulk of ions carried by the free jet gas expansion would be captured by the dodecapole ion guide structure. After the Mach disk, the flow undergoes a series of expansion and compression waves as it travels down the D Jet ion guide. The internal taper of the ion guide helped to focus the gas and ion beam to the exit aperture. These results showed no indication of a pressure increase in the vicinity of the IQ00 lens, and this suggests that the impact pressure was minimal.
Simulations were conducted by combining the CFD solution with electrostatic field modeling using a previously described approach to estimate ion transmission efficiency with this configuration. Briefly, the simulations involved two key components, a Laplace solver (Rx) and a trajectory calculator (Sx). The Rx solver calculated the potential at regularly spaced grid points, and the Sx calculator incorporated the CFD solution in addition to the electrostatic modeling. The favorable flow fields resulting from the shape of the D Jet ion guide and the electrical containment from the RF field applied to the dodecapole resulted in greater than 90% transmission from the orifice to the Q0 region for ions with m/z of 195 and 609.

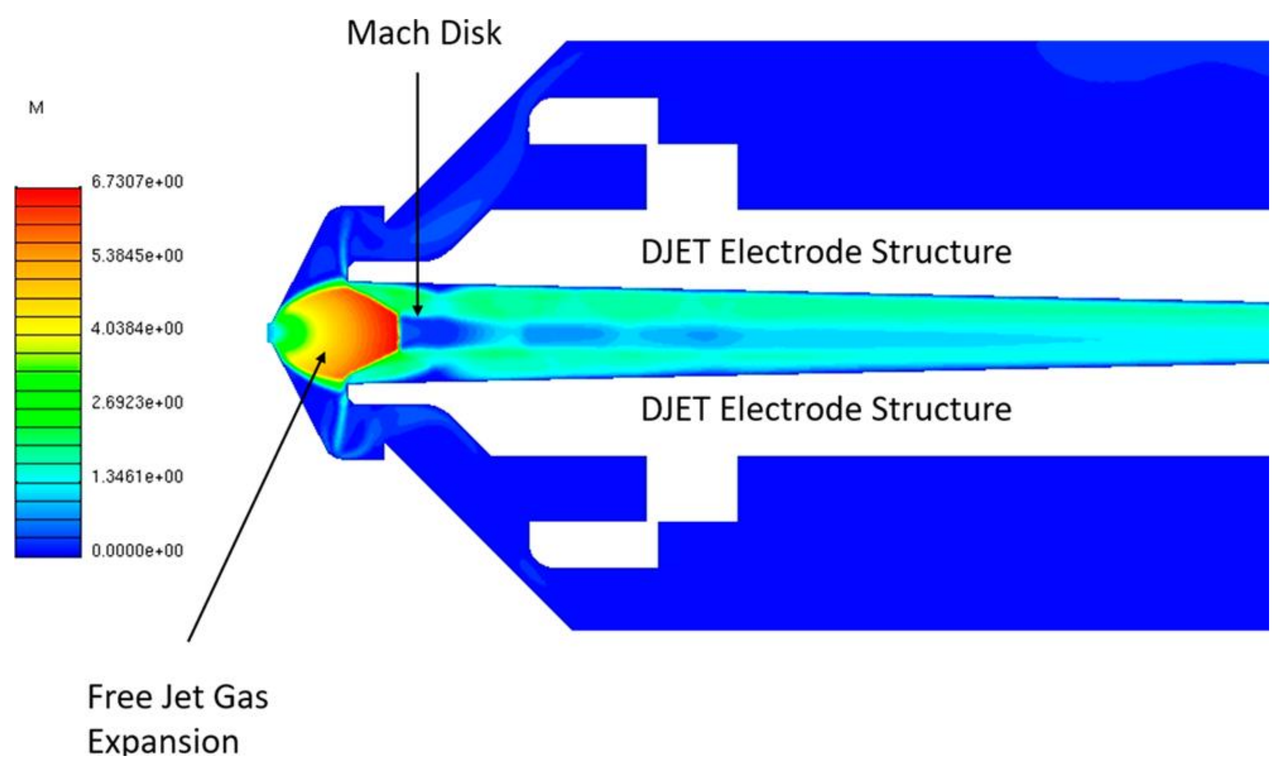

Figure 2. CFD modeling of the gas flow in the D Jet ion guide.

ION TRANSMISSION

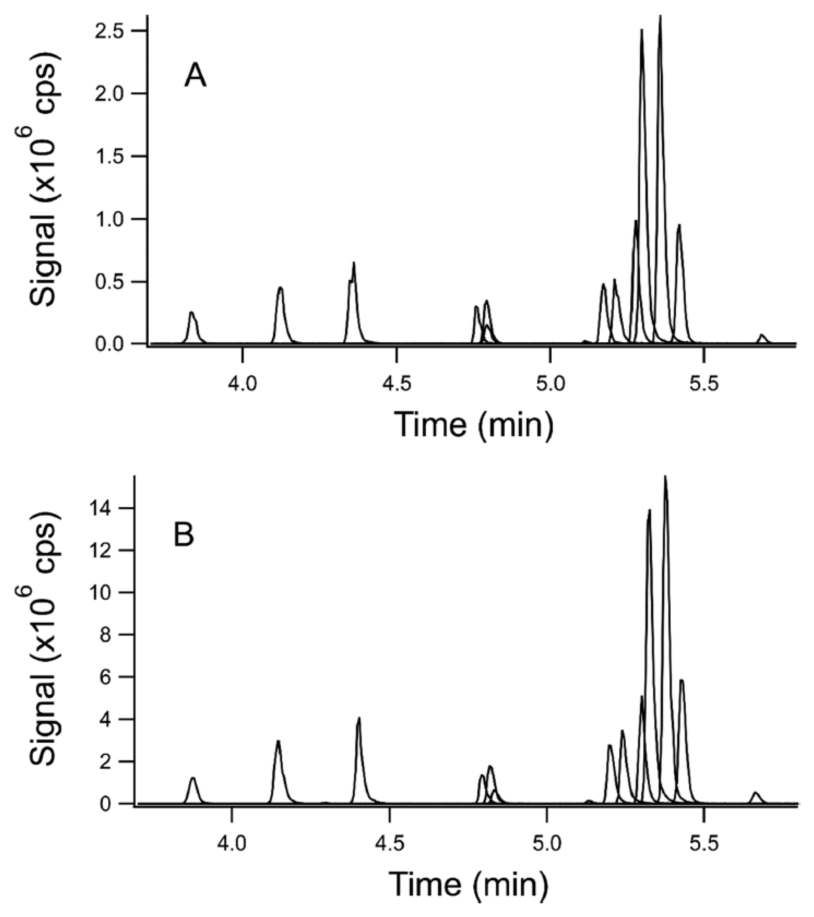

Figure 3. LC-MS chromatograms for a 12-compound mixture taken in the positive ion mode using a standard SCIEX 6500+ system MS inlet (A) and the prototype D Jet ion guide inlet system (B).

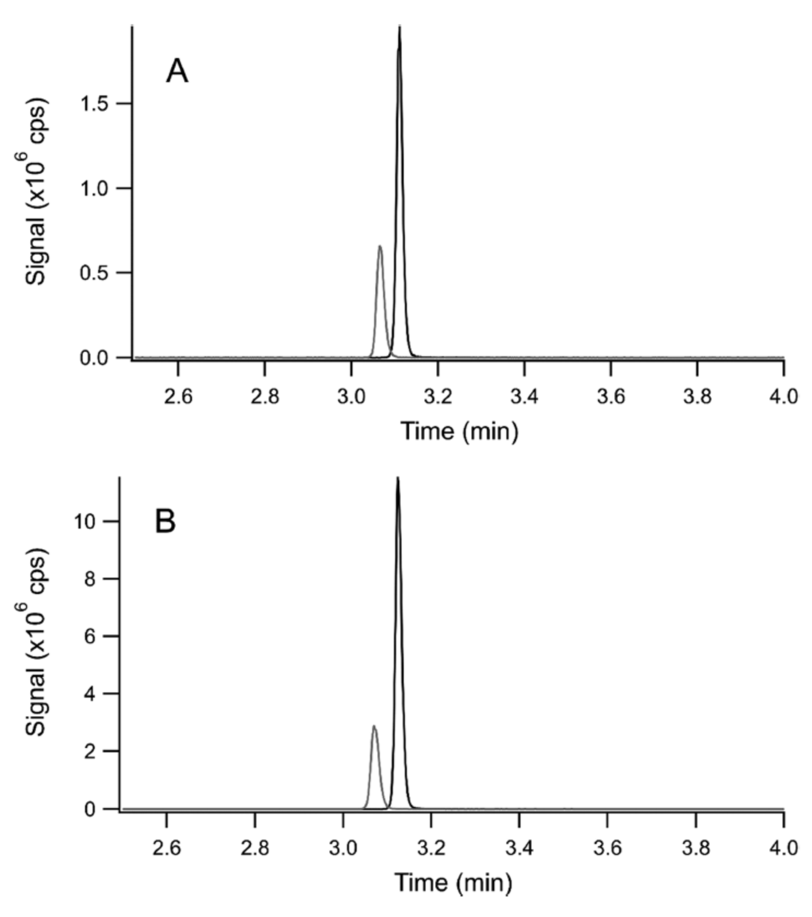

Figure 4. LC-MS chromatograms for a 2-compound mixture taken in the negative ion mode using a standard SCIEX 6500+ system MS inlet (A) and the prototype D Jet ion guide inlet system (B).

As shown in Figures 3 (positive ion mode) and 4 (negative ion mode), the combination of the larger inlet orifice and the effective ion transfer properties of the D Jet ion guide gave signal increases on the order of approximately 5.5X.

DECLUSTERING IN THE Q0 REGION

A small DC potential difference between the IQ0 and the Q0 rodset is sufficient to provide effective declustering in the Q0 region. In cases where the ion of interest is more resilient to thermal heating than background interferences, it is possible to improve S/N

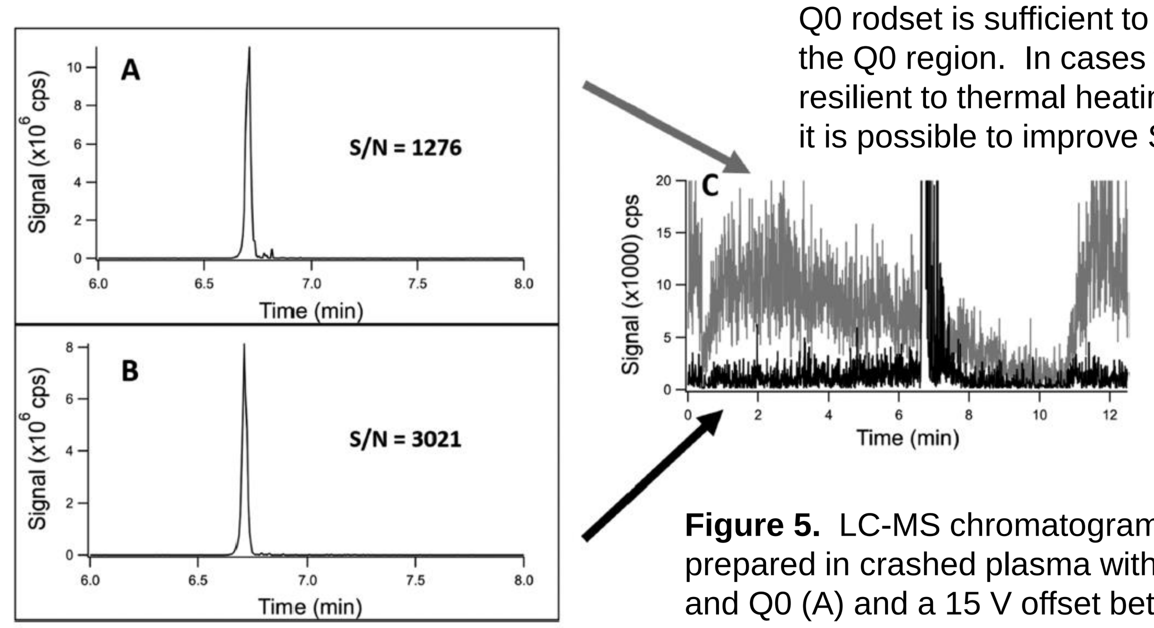

Figure 5. LC-MS chromatograms for a sample of prazepam prepared in crashed plasma with 0 V offset between the IQ0 lens and Q0 (A) and a 15 V offset between the IQ0 lens and Q0 (B). An overlay of the MRM traces is also provided (C)

ROBUSTNESS AND CONTAMINATION

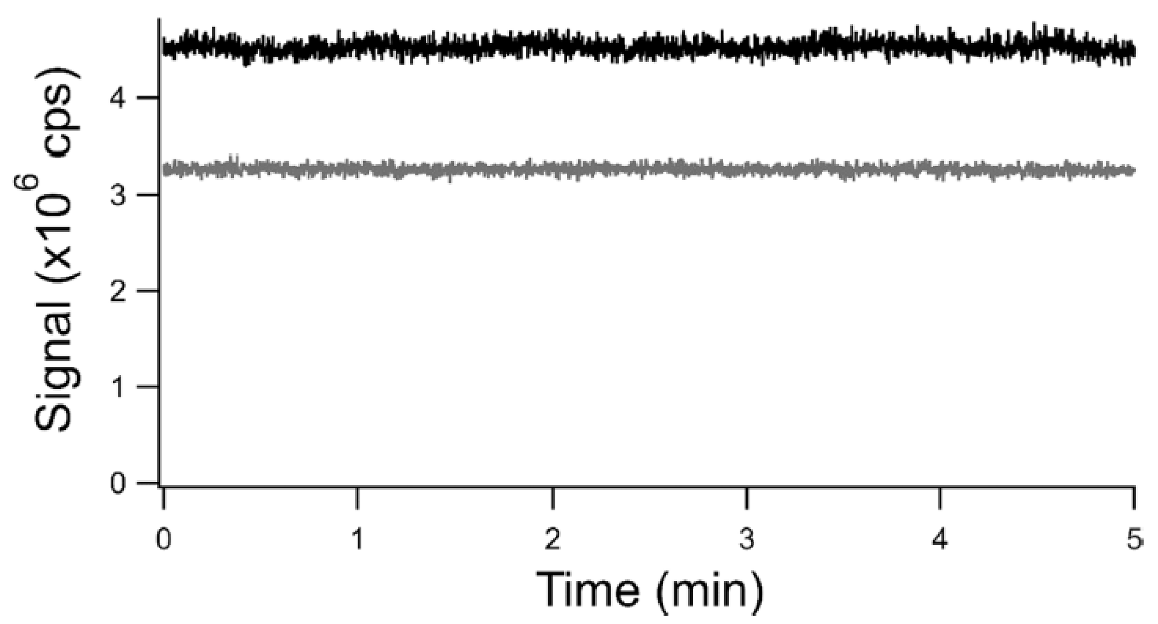

Figure 6. MRM signal decay measured during a highly accelerated contamination test using a mixture of extracted tea and arugula with the high gas conductance inlet. The black trace corresponds to the baseline signal (4,544,266 +/- 73,795 cps) and the gray trace corresponds to the signal measured after infusing 80 mL of matrix (3,268,030 +/- 43,277 cps).

Robustness to contamination is a key attribute for triple quadrupole mass spectrometers. In the present context, robustness refers to the ability of the mass spectrometer to maintain long-term performance under exposure to large volumes of complex sample matrices. The prototype interface described in this poster improves sensitivity by transferring a larger portion of the ions into the vacuum system and therefore concerns related to robustness might be valid. Therefore, a highly accelerated robustness test was run on both the novel D Jet ion guide configuration and a standard SCIEX 6500+ system. The signal reduction was 28% for the D Jet ion guide configuration and 34% for the SCIEX 6500+ system, confirming that the novel configuration provides similar robustness characteristics to the lower gas throughput system.

CONCLUSIONS

A new dodecapole ion guide has been designed to more effectively capture ions from high gas load atmosphere to vacuum ion sources. In combination with two additional differentially pumped quadrupole ion guides, the D Jet ion guide increases the ion transmission efficiency over a two-stage differentially pumped interface. An increased number of ions are transferred from the ion source using a larger inlet orifice, and scattering losses in the shock waves of the accelerating gas beam are minimized to yield a signal improvement on the order of 5.5 ×. Efficient declustering or fragmentation in the third differentially pumped region enables reduction of chemical noise from background clusters. It also enables generation of fragment ions that can be further fragmented in the downstream collision cell for pseudo-MS3 experiments, albeit without mass selection in the first stage. The dodecapole ion guide has exhibited a resistance to loss of performance due to contamination effects, such that other factors such as inlet and Q1 contamination provided more of a limitation in long term robustness experiments.

TRADEMARKS/LICENSING