Coupling Atmospheric Pressure Optics with Field-Free Ionization Sources

Edward Sheehan[1], Ross Willoughby[1], David Fries[2]

[1]Chem-Space Associates, Pittsburgh, PA; [2]U. South Florida, St. Petersburg, FL

High electric potentials associated with most commercial ion sources, such as APCI and electrospray, can have efficiencies less than 0.01% with over 99% of the source current lost before ions enter the vacuum system. These loses primarily occur in the source chamber due to the dispersive flow and electric fields from the ionization process, and diffusion. To minimize theses loses and establish a consistent response, all AP nebulizers (APCI and ES) are designed to be closely coupled with the sampling aperture; with individualized distance between the nebulizer and opening, a range of gas flows, both concurrent and counter current, a range of electric potentials, optics in the ionization chamber, heat input, and a range of liquid flows. We refer to this optimization of the AP sources as being "sweet-spotted".

We present here remedies, such as, field-free ion sources, for electrospray and APCI in combination with ion optics and viscous flow to eliminate these dispersive electrical forces and deliver ions into apertures and the opening of tubes leading into mass spectrometers

Forces at Atmospheric Pressure Leading to Dispersion of Ions from AP Ion Sources

Table 1 summarizes the forces that influence the motion of ions at atmospheric pressure. Diffusion (see Figure 1) dominates the motion of ions in a field-free region. Electrostatic fields provided by ion optics can overcome diffusion and be used to direct and focus ions present in field-free regions into apertures and the tubes (Figure 1). In addition, bulk flow at the openings of tubes and apertures can be used to overcome the dispersion that takes place as ions enter tube and flow into the relatively field-free environment of the interior of tubes.

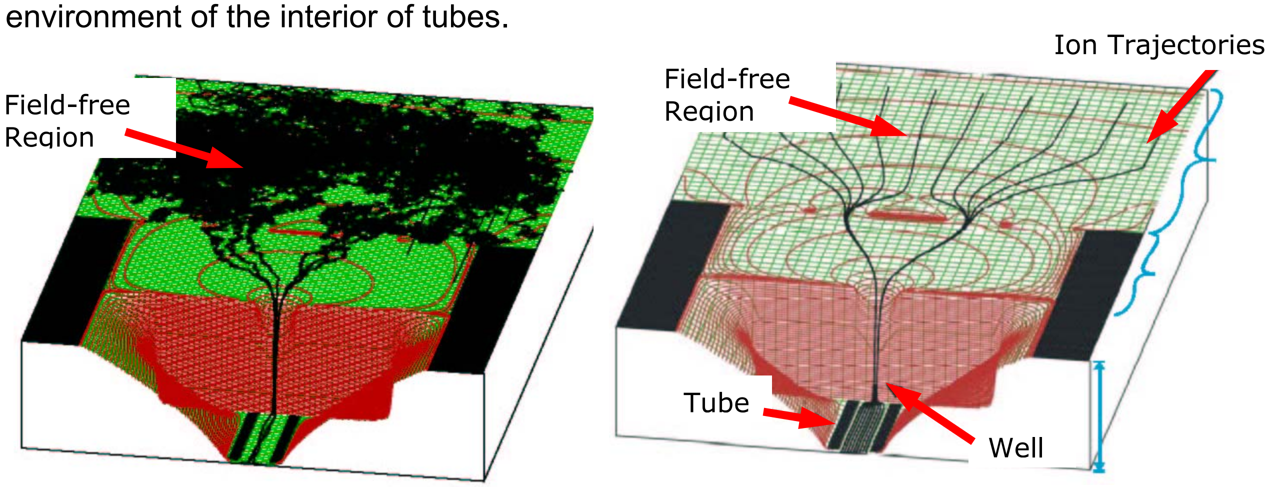

Figure 1 (left) The motion of ions in a field-free region is dominated by diffusion in the absence of electric fields or viscous flow of gases. (right) Simulation showing ion trajectories without considering diffusion.

Table 1 Forces at Atmospheric Pressure that Influence the Ability to Focus Ions.

Force	Comments
Diffusion	• Always present. • Dominates the motion of ions and neutrals in low field and low flow regions. • Leads to loss of ions near surfaces: inside of ionization chambers and tubes.
Electric Potential	• Can overcome diffusion. • Move or direct ions based on their mobility in an electric field. • Dispersive electric potentials from ionization sources can lead to loss of ions inside of ionization chambers and at the entrance to tubes. • Ion Optics can be used to focus and direct ions. • Deep electrostatic wells can collect ~100 % of the ions from ionization chambers.
Bulk or Viscous Flow	• Can overcome diffusion. • Move or direct both neutral and ionic species in a bulk fashion. • Used in combination with ion optics ions collected at the bottom of electrostatic wells can be directed into and through tubes.

<u>Conclusions</u>

The observed collection efficiency for both ES and APCI field-free sources in these studies resulted in 80-100% ion collection efficiency to the bottom of the well. To qualify these results, it should be noted that in some cases over 5 kilo-volts at the bottom of the well was required to yield high efficiencies; but at a high cost. The deeper the well (the higher the potential) more ions are collected but more ions are lost at the entrance due to the defocusing electrostatic fields at the opening. These forces can be diminished or overcome by a combination of matching the diameter of the tube to the cross-section of the focused ion beam (2-4 mm) and increasing the flow of gas (~10 LPM) into the opening. Once ions enter a tube there is very little loss to walls; and ions can be delivered to smaller openings (i.e., a single aperture, tube, an array of openings) at the end of the tube.

<u>References</u>

- Atmospheric Pressure Ion Optic Patents for E.W. Sheehan and R.C. Willoughby: 6,744,041 (June 1, 2004); 6,818,889 (Nov. 16, 2004); 6,949,740 (Sept. 27, 2009); and 7,081,621 (July 25, 2006).
- Remote Reagent Chemical Ionization/Electrospray Source patents for E.W. Sheehan and R.C. Willoughby: 6,888,132 (May 3. 2005); 7,095,019 (Aug. 22, 2006); 7,253,406 (Aug. 7, 2007) and pending.

<u>Acknowledgements</u>

- NIH (Grant RR019811401A1)