Simulation of Ion Trajectories in an Ion Mobility Spectrometer for Atmospheric Pressure Plasma Diagnostics

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1. Introduction

Ion Mobility Spectrometry (IMS) has been used in the analysis of explosives, and dangerous narcotics. The process involves the measurement of the electrical current signature of ions in a buffer gas under an applied weak electric field. Depending upon the mobilities (K_0) of ion species present in the swarm, the time evolution of the signal shows characteristics of the ion time-of-flight. Recently, the application of this method has been expanded to analyses of large biomolecules [1].

The transport of ions in an IMS drift tube is determined from the collisions of ions with the background gas molecules. A simulation model of the ion trajectory inside the spectrometer is being developed to estimate the mass resolution of the system.

2. Target Device

A 13.56 MHz RF driven Ar AP plasma torch serves as the ion source for the 5 cm long IMS. The trajectory of Argon ions is simulated as they move through the IMS device (Fig.1). The device realizes a constant electric field at the center to which a background gas of air at 273 K, and 760 Torr interacts with the moving ions.

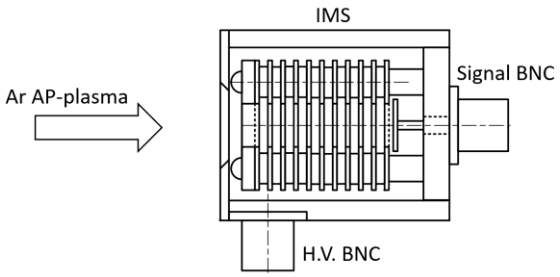

Figure 1. Schematic diagram of the IMS device.

The path of the ions was calculated using the motion of an ion in a uniform electric field, and the collisional model of rigid spheres using the Monte-Carlo method which assumes that the collision between an ion and a gas molecule will result to the equal likelihood that the ion will be scattered in any given direction in the center-of-mass coordinate system [2]. The details of the calculations of velocity transformations and collisional probabilities are based upon the research of Xu, and Whitten [3].

3. Preliminary Results

The trajectory of a single Ar^+ ion moving through the IMS was calculated using Visual Basic Studio in C# (Fig.2) with a time step of 30 ps as utilized by Xu, and Whitten in their study [3].

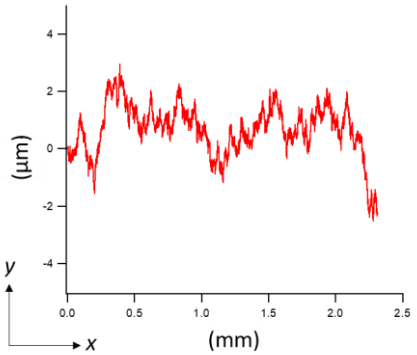

Figure 2. Trajectory of an Argon ion in the IMS with an x-axis of up to 2.5 mm, and a y-axis ranging from -5 μm to 5 μm.

The ion was made to travel over a period of 30 μs. Further computations of the swarm will be done to estimate the dispersion of the time-of-flight signal which would then be directly compared to experimental data.

4. References

[1] Harvey, S. R., MacPhee, C. E., Barran, P. E. Methods (2011) 54: 456–461.
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[3] Xu, J., and Whitten, W. B. Int. J. Ion Mobil. Spec. (2008) 11:13–17.