Simulation of Differential Ion Mobility (DMS) Principle Coupled with Mass Spectrometry in Atmospheric Pressure

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Abstract

Mass spectrometry is an analytical technique widely used in the scientific community to determine chemical composition of sample compounds. Typically, mass spectrometers perform their analysis under vacuum conditions, though atmospheric pressure mass spectrometers are becoming more prevalent. With the development of atmospheric pressure mass spectrometers, techniques such as FAIMS (Field Asymmetric Ion Mobility Spectrometry) have emerged; which achieve higher transfer efficiency into the mass spectrometer and thus improve the instrument's sensitivity. Ion behavior in higher pressure conditions, such as in ambient ionization sources, is less understood, thus making it more difficult to predict ion trajectories and concentrations. Modeling of this ion behavior becomes challenging, due to concurrent effects of fluid flow and diffusion in addition to dynamically changing electric fields. These non-linear parameters are however, more easily employed in current software iterations. Ion behavior for Cesium is modeled using two simulation programs, COMSOL Multiphysics and SIMION®. Specific compound parameters, including ion mobility coefficient in low fields and alpha parameters, are obtained experimentally. These serve as inputs to define ion behavior in both software packages. Ion trajectory is dependent on several factors, consisting of convection forces due to air flow, migration forces due to high voltage oscillating fields and diffusion forces due to particle-to-particle interaction in atmospheric pressure. Specifically during COMSOL modeling, three dependent modules including electric current, laminar flow, and transport of diluted species are incorporated. Numerical solutions are calculated across a 2D model using a fine mesh that encompasses three domains. The first domain represents the DMS plates, in which a bisinusoidal AC waveform is applied. The second domain is an air gap, where no electric potential is employed. The third domain is defined as the MS capillary inlet, where a DC potential exists. COMSOL alternatively offers a Particle Tracing Module which solves particle motion through Lagrangian mechanics. This newly introduced COMSOL module allows for faster computing while also permitting individual ion tracking. Unlike the transport of diluted species module, the Particle Tracing Module does not incorporate diffusion effects. Both COMSOL Multiphysics and SIMION present several features, and a head-to-head assessment of both packages will be performed and compared to experimental results. Experiments will entail the collection of data for inorganic radionuclide analogs such as Cesium. Optimization of the DC compensation voltage for filtering of each ionic species will be performed through the simulation software, and the total ionic current for each species from the models will be validated with the

experimental tests. It is expected to obtain sensitivity and resolution information due to varying parameters such as electric field frequency and amplitude and ion inlet velocity. This modeling is being used towards potential forensic analysis of radiological dispersion devices (RDDs) also known as dirty bombs. Additionally, parameter optimization through simulations can be used as a guide for the design of a field deployable mass spectrometer.