

High resolution mobility spectrometry in a co-axial platform

September 2023

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Abstract

Ion mobility spectrometry is an analytical technique that separates ions in the gas phase based on their interaction with a neutral buffer gas. Ion mobility spectrometry performs separations quickly (typically less than a second) and the ion mobilities are very reproducible across different laboratories. This project aimed at evaluating the performance of a new ion mobility device. The new device relies on conducting ion mobility separation in a curved geometry. The project explored the operation landscape of the device using ion trajectory simulations then fabricated and experimentally demonstrated the device's performance. Ion trajectory simulations on a set of tetraalkylammonium and phosphazene ions indicate that ions traveling a curved path length undergo mobility separation that is similar to a straight path. The ion mobility resolution of the curved device was found to be similar to that of a straight path of a similar length. The experimental validation of the new device confirmed the device's ability to separate ions according to their mobilities. Sets of mixtures (tetraalkylammonium ions, phosphazene ions, and peptide ions) were evaluated for separation and transmission.

Summary

This project evaluated the performance of a novel ion mobility device that has a curved architecture. The device's geometrical and operational parameters were investigated using ion trajectory simulations to aid in finding the optimum parameters. The fabricated device was assembled and evaluated in conjunction with a mass spectrometer. The experimental results indicated a good performance on par with ion mobility devices of conventional linear paths.

Acknowledgments

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Acronyms and Abbreviations

QTOF: Quadrupole time of flight

MS: Mass spectrometer

IMS: Ion mobility spectrometer

i.d.: inner diameter

ADC: Analog-to-Digital Converter

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1.0 Introduction

Efforts to increase the resolving power of ion mobility beyond the current limitations require increasing the path length either physically or effectively. Effectively increasing the path length through cycling ions over the same path length can increase the resolving power but for a narrow range of mobilities. Physical increase of path length was achieved through a serpentine path or stacking of multiple Structures for Lossless Ion Manipulations (SLIM) modules. These successful SLIM devices still occupy some footprints. With the maturation of 3D printing and flexible printed circuit board technologies, it is becoming more feasible to design novel ion mobility devices that provide an extended path length while maintaining a compact footprint making these devices more adaptable to miniaturization and seamless integration to commercial mass spectrometers. One such design takes advantage of curved surfaces to form an ion manipulation conduit having a serpentine or a helical pathway for extended ion mobility separations. Performing mobility separation in curved pathways can be challenging due to the race-track effect that degrades the separation quality of the device. The race-track effect happens when ions on the outer side of the curved track travel longer distances than ions on the inside of the curved track. The race-track effect leads to peak broadening and loss of resolving power. In this project, we developed and evaluated the performance of a novel ion mobility device of a curved geometry. The new device featured tracks that were both curved and zig-zagged. The device design and operating parameters were evaluated and optimized using ion trajectory simulations. The new device was evaluated experimentally in conjunction with a Time-of-flight mass spectrometer.

1.1 Ion Simulations & Experiment Setup

Ion trajectory simulations were performed using SIMION 8.1 software and utilizing the statistical diffusion simulation user program. 1000 ions of tetraalkylammonium cations (a range of m/z 242-466) and phosphazene cations (a range of m/z 622-1822) were used for the simulations. The device was operated at a pressure of 2.5 Torr of nitrogen. The arrival times of ions were recorded and compared. Experiments were performed using an electrospray ionization source where formed ions were injected into an inlet capillary heated to $\sim 120^\circ\text{C}$. Ions exiting the inlet capillary were focused using an ion funnel operating at a pressure of 9-10 Torr. The focused ion beam was then transmitted and trapped inside an ion funnel trap operating at a pressure of ~ 2 Torr. Trapped ions were released from the ion funnel trap into the ion mobility device held at a pressure of ~ 2 Torr of nitrogen. Ions exiting the novel ion mobility device were captured by an ion funnel that focused the beam into a 2.5 mm i.d. conductance limiting orifice. The focused ion beam entered the interface of an Agilent 6538 QTOF MS and was detected using a multichannel plate detector. The signal from the QTOF detector was routed into an 8-bit ADC and processed using a home-built acquisition software.

2.0 Results

2.1 Ion trajectory simulations

Two ion mobility devices were compared: a conventional linear track and curved track (Figure 1). All ions of all m/z values were flown for about 2 meters to have arrival time distributions that are more realistic. For the linear track the tetraalkylammonium cations (m/z 242-466) arrived in about 15-90 ms. The peaks had arrival time distribution of standard deviations that ranged from 0.3 ms for the fast ions to \sim 0.5 ms for the slow ions. The curved track produced similar results in terms of the arrival time distributions and their standard deviations which indicate the curved track has minimal effect on the resolving power of the device.

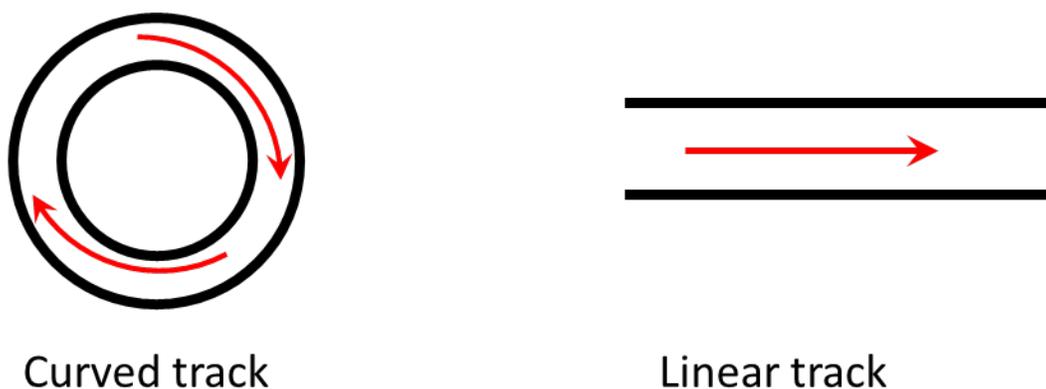


Figure 1. Schematic diagram of the curved and linear tracks. The arrows indicate the direction of ion motion inside the device.

2.2 Experimental results

Experiments were performed on the curved ion mobility track created by two surfaces. The potentials applied to the two surfaces manipulate the ion motion in a way that causes ions to separate according to their velocities (i.e., mobilities). We first confirmed the ability of the device to transmit ions of a broad m/z range (200-1800) as well as its charge capacity (we were able to transmit ion current on the order of a few hundred milliamperes). Experiments on the phosphazene ions revealed that injecting a pulse of ions into the IMS device resulted in arrival time distributions that are ranked according to ions mobilities where ions of high mobilities arrive at a shorter time than ions of low mobilities. We observed that ions of high mobilities produced sharper peaks than those of low mobilities (see Figure 2). We also observed that ions of low mobility (i.e., peaks of longer arrival times) have asymmetric shapes compared to those at shorter times. This may indicate that ions of low mobilities are experiencing inhomogeneous electric fields compared to ions of high mobilities. It is possible that shaping the electric field can make the peak shapes more symmetric. The average IMS resolving power of the new device was measured to be \sim 53 which we believe can be increased by optimizing the electric field by shaping the voltage applied and/or the electrodes geometries.

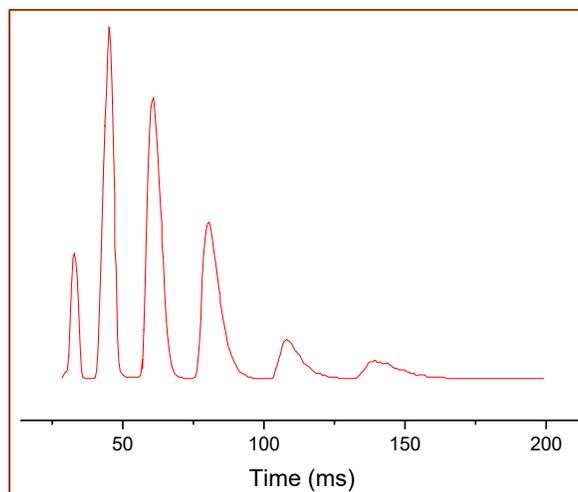


Figure 2. Arrival time distribution of a mixture of phosphazene cations.

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