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Simulation of Electric Potentials and Ion Motion in Planar Electrode Structures for Lossless Ion Manipulations (SLIM)

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Abstract

We report a conceptual study and computational evaluation of novel planar electrode Structures for Lossless Ion Manipulations (SLIM). Planar electrode SLIM devices were designed that allow for flexible ion confinement, transport and storage using a combination of RF and DC fields. Effective potentials can be generated that provide near ideal regions for confining and manipulating ions in the presence of a gas. Ion trajectory simulations using SIMION 8.1 demonstrated the capability for lossless ion motion in these devices over a wide m/z range and a range of electric fields at low pressures (e.g. a few torr). More complex ion manipulations, e.g. turning ions by 90° and dynamically switching selected ion species into orthogonal channels, are also shown feasible. The performance of SLIM devices at ~4 torr pressure for performing ion mobility based separations (IMS) is computationally evaluated and compared to initial experimental results, and both of which are also shown to agree closely with experimental and theoretical IMS performance for a conventional drift tube design.

Keywords

Gas phase ions; lossless manipulations; ion trajectory simulations; ion mobility; resolving power

Introduction

Gas phase separation techniques such as Ion Mobility Spectrometry (IMS) coupled to Mass Spectrometry (MS) have a broad potential for improved analyses particularly for biological applications involving ‘pan-omics’ measurements [1, 2]. As the sample complexity increases, the potential benefits from applications of high-resolution separations and more complex sequences of ion manipulations in conjunction with such analyses also increases. However, the use of extended sequences of ion manipulations comes at the expense of significant instrumental complexity, cost, and sensitivity constraints due to ion losses, to the extent that such approaches extending beyond a few simple steps have been effectively impractical, and thus broadly ignored.

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Ion losses (e.g., due to neutralization, contact with surfaces, limited transfer efficiency through interfaces... etc.) have long been a challenge for mass spectrometry. Typically, only a small fraction of the ions generated by an ion source actually reaches the m/z analyzer region of the mass spectrometer [3, 4], and the use of more extensive gas phase separations would tend to further aggravate this situation, despite the attractions of e.g., fast gas phase ion separations. Electric fields, gas dynamic effects, and their combination have been used to mitigate such issues, particularly with higher pressures ionization methods such as ESI. In the intermediate pressure region of, e.g. ESI-MS interfaces, electrodynamic ion funnels [5] have served to greatly increase ion utilization efficiency by providing effective ion confinement, focusing and transport over a significant m/z range. In addition, electrodynamic multipole ion guides and stacked ring electrodes have been e.g., used for efficient transfer, to construct drift cells, and to effect mobility based separations [6] in conjunction with MS. Several other works have also demonstrated the use of radiofrequency (RF) confining fields for confining and transporting ions. Work by Masuda et al. in the 1970s and 80s led to development of so called ‘electric curtain’ devices that used travelling wave (TW) fields for ion transport, and application to the study of aerosol particles [7], and biological cells [8], among others [9]. The RF ‘ion carpet’ [10–13], and ion surfing [14] devices are other examples of devices that have been used to perform ion manipulations by using RF confinement. Other types of ion manipulations, such as confinement (i.e. trapping) for extended periods, gas phase reactions, and the transfer or ‘switching’ of ions selectively between spatial regions, are also attractive for the development of more sensitive and faster analytical measurements. But the development of significantly more complex sequences of manipulations requires new approaches to the design of ion optics that are more efficient and less cumbersome.

In this spirit new Structures for Lossless Ion Manipulation (SLIM) are being developed at our laboratory with the intent of enabling much more sophisticated gas phase ion manipulations, including ion mobility separations. SLIM devices use RF and DC potentials applied to arrays of planar electrodes (each having dimensions typically on the order of millimeters) on surfaces, to confine and manipulate ions (in this work at pressures of few torr) in a potentially lossless fashion. SLIM components with electrode arrangements can be fabricated to enable specific manipulations, and then be assembled into more complex modules and larger devices (e.g., integrating multiple modules) to perform complex sequences of manipulations, as needed for the specific application. Initial SLIM components being evaluated include: (a) a straight drift section; (b) a 90° turn drift section; and (c) a “switch” to direct ions along one of two designated paths. We envision that these components will serve as the building blocks for much more complex SLIM modules and devices, similar to the basic electronic components (e.g. diodes, capacitors, and transistors) that constitute the building blocks of larger integrated electronic circuits.

To develop and refine the design of these SLIM components, as well as to evaluate their performance, a fundamental understanding of the nature of electric potentials and their effect on the ion motion in these devices is essential. In this work, key SLIM components have been explored using computational and ion simulation methods. The nature of the electrodynamic and DC fields used to manipulate the ions in these initial SLIM designs is

reported. In particular, ion motion in the basic SLIM straight drift section has been studied to evaluate its potential performance for ion mobility separations and a range of designs and applied electric fields have been studied to guide the development and the refinement of the respective SLIM component.

Methods

A custom built Matlab (Math Works Inc., Natick, MA, USA) code was used to solve the Laplace equation numerically for key SLIM components. The numerical solver is built upon the finite difference method and second order central differencing scheme for discretization [15]. The net potential (ϕ) experienced by an ion with mass (m) and charge (q) in the presence of DC potential (ϕ_{DC}) and RF (ϕ_{RF}) potential with frequency (ω) was extracted from the solution to the Laplace equation, using the well-known pseudo potential well

approximation equation [16]: $\phi = \frac{q}{4m} \frac{|\nabla \phi_{RF}|^2}{\omega^2} + \phi_{DC}$. Ion trajectory simulations were performed using SIMION 8.1 (Scientific Instrument Services Inc., Ringoes, NJ, USA). The 2D geometry for one surface of the SLIM components was constructed in SIMION workbench, and planar symmetry was used to define the second parallel set of electrodes. The CAD geometry files for the electrode arrangements and dimensions used to construct the actual SLIM components (details to be reported elsewhere) [17] were imported into SIMION to enable comparison of the present simulations with the experimental measurements. The SLIM electrodes were assigned corresponding voltages using the ‘fast adjustable electrode’ feature in SIMION, which allows rapid field variation during ion motion [18] to account for the RF fields applied. The individual electrodes were assigned DC and time varying RF potentials. User programs were incorporated into the simulation to allow collisions with the buffer gas using the statistical diffusion simulation (SDS) [19] model. The SDS model accounts for both the ion mobility-based drift (using Stoke’s Law) and the random diffusion (using tabulated collision statistics and randomized ion jumps). [19–21] The SIMION SDS model was previously used to study the ion motion in viscous environments (low E/N scenarios), and the pressure used here (~4 torr) corresponds to a viscous regime for the drift of ions at the applied fields (~20 V/cm). Thus, the SDS model simulations are expected to effectively represent ion drift and diffusion statistics. Each simulation run consisted of the trajectories for 1000 ions for each species of interest. All the ions had an initial condition of zero kinetic energy and for simplicity started at a point source at the entrance of the SLIM device.

Figure 1 illustrates aspects of the SLIM designs, the electrical potentials applied, and the coordinate scales used for the computations and simulations. The Z-axis is designated as the direction of the intended ion motion in the linear SLIM component illustrated. The central ‘rung’ electrodes are arranged sequentially along the Z-direction with alternating RF phase between each electrode and a DC voltage gradient to drive ion drift motion. The rung electrodes are flanked on either side by “guard” electrodes in the XY plane. A DC potential with a small positive bias (in the case of positive ions) to the voltage on rung electrodes is applied to the guard electrodes. Two such planar electrode boards arranged in parallel, at an inter-board gap (5 mm in this study) define the SLIM component. The RF and DC potentials

applied to the electrodes on these surfaces are expected to both confine the ions in two dimensions and produce ion drift motion in the other dimension between the two surfaces.

The width of the guard electrode used in this work was 5.9 mm, width of the central rung electrodes was 0.76 mm, and the gap between electrodes was 0.76 mm (Figure 1b). Thus, for every guard electrode there are four corresponding rung electrodes. (While a single guard electrode per every rung electrode would generate somewhat smoother potential profiles, we simplified the design of the initial components fabricated to reduce the number of electrodes and electrical components.) To bias the guard electrode relative to the rung electrodes, we used the rung electrode having the highest potential as the reference point (see Figure S1 for relative voltage assignment for rung and guard electrodes).

For experimental measurements ions were generated using an Agilent Tuning Mix (Agilent Technologies, Santa Clara, CA, USA) directly infused at 300nl/min and to an electrospray source using an applied potential of 2500 V. Charged particles passed through a 500 μm i.d. stainless steel capillary heated to 120 $^{\circ}\text{C}$ into an ion funnel trap [22, 23], where they were accumulated for 1 ms, and trap exit gate pulses of $\sim 162\ \mu\text{s}$ width were used for ion injection into the SLIM device. The SLIM device and rear ion funnel were maintained at 4.10 torr of nitrogen gas while the ion funnel trap was maintained at 4.05 torr to establish a positive pressure differential and effectively eliminated the introduction of contaminants to the SLIM device as well as any gas dynamic effects. A constant electric field along the instrument axis was established by a resistive voltage divider. The total length of the SLIM device and rear ion funnel and provided an ion drift length of 63.2cm. The same electric field was maintained through the SLIM device and the rear ion funnel so as not to degrade resolving power. The detailed experimental arrangement is elaborated elsewhere [24].

Results and Discussion

To study the effectiveness of the electrode configurations and applied fields for ion confinement and ion drift in the SLIM module, effective potential calculations were made using solutions to the Laplace equation as well as ion trajectory simulations using SIMION 8.1. The Laplace equation was solved with appropriate RF and DC boundary conditions (Figure 1c and Figure 1d). The voltage applied to each central electrode is defined as $U_{\text{DC}} - (n-1) dU + (-1)^n V_{\text{RF}}$; where n is the electrode number, U_{DC} is the DC voltage applied to the first rung electrode, dU is the DC voltage drop across two adjacent electrodes and the V_{RF} is the amplitude of the applied RF waveform (0-peak). The voltage applied to the guard electrodes is $U_{\text{DC}} + U$; where U is the DC bias applied to guard electrode relative to the first corresponding rung electrode. Rung electrodes with a length of 10 mm in conjunction with RF voltages of 200 $V_{\text{p-p}}$ were initially considered. A DC voltage drop of 60 V was applied across a series of 12 rung electrodes over a length parallel to the XZ plane. The guard electrodes were biased by 5 Volts above the first rung electrode. Figure 2a and 2b show the contours and profile of the potential well between the SLIM component surfaces in the YZ and XY planes, respectively. In XY plane, symmetric trapping well region is clearly identified in the potential profile, demonstrating the ability of SLIM devices to effectively confine ions. The YZ plane linear potential drop and constant electric field at the center of the trapping well illustrates the potential for ion drift motion in conjunction with lossless ion

transmission. In the YZ plane, along a line away from the center axis (and closer to the RF electrodes), the potential profile shows axial trapping wells in conjunction with a linear drift field.

To further evaluate the potential for this SLIM component to effectively confine and transmit ions without losses, SIMION simulations were performed for conditions of 4 torr pressure at 298 K. The trajectories in a SLIM linear component for a group of ionic species with m/z values 118, 322, 622 (reduced mobility $K_0 = 1.17 \text{ cm}^2/\text{V.s}$), 922 ($K_0 = 0.97 \text{ cm}^2/\text{V.s}$), 1222 ($K_0 = 0.85 \text{ cm}^2/\text{V.s}$), and 1522 ($K_0 = 0.73 \text{ cm}^2/\text{V.s}$), major ions from an Agilent Tune Mix, were simulated using SIMION. In addition, to further evaluate the m/z range of operation for SLIM, the trajectories of representative ions with m/z 50, 75, 100, 2000, 3500 and 5000 were simulated. For the representative ions, the ion diameter (d_{ion} in nm) and reduced mobility (K_0 in $\text{cm}^2/\text{V.s}$) values were estimated by the SDS model from their ionic masses (amu) in SIMION using its provided relationship estimation [19, 21]. The initial conditions of the ions in the simulation were defined as a point source at the beginning of the SLIM device and equidistant from the two parallel SLIM boards. The initial ion kinetic energy was set at 0 eV since at 4 torr ion motion is damped and thermalized by gas collisions on a nano-second time scale [25]. Subsequent ion motion is governed only by the drift field imposed in the SLIM device. Also the ion injection into the SLIM device occurs via an ion funnel trap that focuses the ion beam to a relatively tight packet with a narrow spatial distribution. Our experimental design aims to achieve negligible dynamic effects in the ion funnel and SLIM interface regions [22–24, 26], and this is assumed for this study.

The m/z range of the SLIM component for lossless transmission is determined by factors that include the applied RF and DC potentials, the geometry of the electrodes as well as the pressure, and simulations can be used to guide all aspects of the SLIM design, as well as the design of components for other manipulations. Figure 3a inset shows the ion trajectories in the XZ view planes in the SLIM component. The percentage of ions transmitted versus m/z is shown in Figure 3a, with the identified low and high mass ranges of operation. The approximate high m/z cutoff for lossless transmission with the current parameters (RF 200 V_{p-p} 0.8 MHz, 20 V/cm DC gradient) was ~2500, beyond which the efficiency of transmission drops below 100% due to less effective confinement. The low m/z cutoff was more abrupt; while 100% transmission was observed at m/z 50, significant loss of ion signal was observed at m/z 25 due to ion instability in the RF trap. Between m/z 50 and m/z 2500, the ion transmission was 100%.

Other SLIM components have been designed for incorporation into modules enabling more complex ion maneuvers. The ion trajectory simulations for a SLIM “elbow” (i.e. 90° turn) (Figure 3b top panel) and a “tee” (Figure 3b bottom panel) components also showed the potential for 100% ion transmission efficiency. The SLIM “elbow” and “tee” were built using the same geometries of electrodes as the straight section (0.76 mm thickness of rung electrode, 0.76 mm rung-to-rung electrode gap and 4 rung electrodes per guard electrode). The potentials applied on the electrodes created a voltage drop similar to one applied in the straight SLIM section (trajectories at 20 V/cm drift field, 200 V_{p-p} RF on rung electrodes, 0.72 MHz frequency and 5 V guard bias are demonstrated in Figure 3). The “tee” could be operated in two modes – the “straight-pass” and the “switch”. During the “straight pass”

mode, the switch guard electrode and the switch rung electrode (see Supplementary Information Figure S2) are biased 5 V above the corresponding rung electrode in the straight portion of the device. However, when ions are to be turned, the switch rung electrode was biased to a lower voltage than the adjacent rung electrode in the straight section. In addition, the switch guard electrode was biased to a higher voltage (100 V bias in this case). The voltage gradient in the orthogonal rung section was maintained at that of the straight section of the tee. By dynamically switching between the two (straight-pass and switch) modes ion packets can be selectively switched into orthogonal channels. In the “tee” structure a selected species (m/z 1522, shown as black color trajectories in Figure 3b bottom panel) was selectively switched during a mobility separation into the orthogonal channel while another species (m/z 622, shown as red color trajectories in Figure 3b bottom panel) was allowed to traverse the straight path. This was achieved by dynamically changing the voltage configuration to “switch” mode at the time corresponding to the passage of the m/z 1522 peak through the tee junction (at other times the “tee” operated in the straight-pass mode, preventing ions from turning). Such lossless manipulations allow, for example, switching of selected species to a different spatial region of the device for, e.g., trapping or further ion processing. Additional aspects of the tee, its implementation and application are discussed elsewhere [24, 27]

The ions that are losslessly confined between the SLIM electrodes and surfaces can also be trapped at different locations (between the component surfaces) by using different applied voltages and/or different geometries of electrodes. The depth of the potential well changes with the applied guard bias (Figure 4a), and the electrode dimensions also affect the trapping wells. When the length of the central electrode is reduced (e.g., 3 mm) the field penetration from the DC on the guard electrodes increases. Consequently, the potential well moves away from the axis (see Figure 4b). Moving the potential wells closer to the electrodes can potentially increase the extent of ion activation [28] as ions located closer to RF electrodes experience greater heating [29–33]. Thus, simple modifications of potential and geometries of SLIM devices could provide a flexible platform to create ion traps with controllable trapping capacities and also with potential for populating ions in different regions beneficial for performing ion activation and also ion/ion reactions. Conventionally performing gas phase ion reactions in ion traps requires cumbersome ion optic instrumentation [34–37]. With the ability to dynamically modify the voltages to control trapping well depths and profiles for ionic species, SLIM devices provide a convenient and simple platform for performing complex reactions and controlled manipulations.

The performance of SLIM devices for low field IMS separations was evaluated using simulations and compared to initial experimental measurements (to be reported in detail elsewhere [17]). A 5 mm long central electrode with 5 mm inter-board gap was considered in this case. The arrival time distributions for a peak (m/z 1222), drifting through a single SLIM straight unit were computed at different drift fields ranging from 5 V/cm to 20 V/cm (5 – 15 Townsends). Experimental measurements for the same peak (m/z 1222) were also obtained from a SLIM straight module by assembling six SLIM components (i.e. from twelve SLIM PCBs) and connecting them to mass spectrometer with suitable ion optics, with a total flight path of 63.2 cm (see Methods). The arrival time and resolving power from

simulations corresponded to one SLIM component of 7.7 cm length. Simulating ion trajectories through experimental drift lengths (six straight SLIM units of length 45 cm and additional ion optics) would involve high computation costs for an ion population size providing reasonable ion statistics, hence our approach has been to evaluate the smaller individual SLIM components with results scaled to the geometries of the larger modules used for experiments. The simulated ion time of flight ($t_{simulation}$) and the theoretical ion

time of flight ($t_{theory} = \left(\frac{7.3}{K_o \left(\frac{760}{4} \right) E} \right)$) through 7.3 cm of a SLIM linear component were compared. The theoretical time of flight was calculated using the appropriate ion mobility (K_o cm²/Vs), pressure (4 torr) and electric field (E V/cm) conditions. The simulation and theoretical calculations were in close agreement (Figure 5a).

The simulated peak full width at half maximum (t_{FWHM}) was used to calculate the mobility

resolving power ($r_d = \frac{t_{simulation}}{\Delta t_{FWHM}}$) from simulations performed using SIMION 8.1. A population 1000 ions started from a point source was simulated without space charge effects to evaluate the diffusion limited resolving power through a 7.3 cm SLIM component. The resulting value was used to then compute the diffusion limited resolving power

($R_d = \sqrt{\frac{LEq}{16k_B T \ln 2}} = \left(\sqrt{\frac{63.2}{7.3}} \right) r_d$) of the 63.2 cm design used for experimental measurements. The net resolving power achievable is a combination of the diffusion limited

resolving power (R_d) and the gate limiting resolving power ($R_g = \frac{T}{\Delta T_{gate}}$) [38]. FWHM (t_{FWHM}) of the IMS peak determined the diffusion limited resolving power for all mobilities after a certain ion drift time (T), and the experimental gate opening time (T_{gate}) of 162 μ s determined the gate limited resolving power, specific to mobility of the ion of interest. Ion peak with m/z 1222 was used to calculate the gate limited resolving power from simulations. The net resolving power, also referred to as the conditional resolving power

(R_c), of an IMS device is given by the following equation: $R_c = \frac{R_d R_g}{\sqrt{R_d^2 + R_g^2}}$. The conditional resolving power of m/z 1222 calculated from simulation was in close agreement with the theoretical predictions (Figure 5b). The close agreement of the resolving power to the ideal drift cell theoretical predictions supports the potential utility of SLIM devices for IMS separations, and further confirmed by the good agreement with experimental data (Figure 5b).

Conclusions

Potential calculations and simulations for SLIM components indicate that these devices can allow complex ion manipulations without physical ion losses over a wide m/z range. The trapping capacities and potential profiles in these devices can be altered by the changing electrode dimensions, and can be dynamically manipulated in a controlled fashion using the applied voltages. Ion trajectory calculations show the capability for moving ions effectively around corners, as well as 'switching' ions between different paths. Simulations show that

ions can also be separated based upon their ion mobility in these devices, and with performance close to theoretical for an ideal drift tube, and also consistent with initial experiments (to be reported elsewhere). SIMION simulations are closely aligned with experimental observations, and thus can be used for extensive investigation and design refinement of SLIM component. The predicted IMS device performance (transmission, arrival times, and resolving power) was also robust over a wide m/z range for different applied RF voltages and frequencies. We plan more detailed simulation-driven characterization of alternative SLIM components and refinement of electrode dimensions, voltages, etc., and their influence on performance. These efforts will drive further optimization for their respective SLIM component functionalities, and the design of more complex SLIM modules and devices enabling much more sophisticated ion manipulations.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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Figure 1.

a) SLIM component schematic; b) dimensions of SLIM unit electrodes (L_{ce} range in this study was from 3 mm to 10 mm); c) voltage configuration of SLIM device applied to the central 'rung' electrodes with RF and DC gradient in XZ plane d) voltage configuration on rung and guard electrodes in the XY view plane; U_{DC} is the applied DC voltage on the electrode, V_{RF} is the RF voltage which alternates in phase with adjacent rung electrodes, dU is the DC potential drop from one rung electrode to next, U is the DC bias voltage applied to the guard electrodes.

a)

b)

Figure 2.

a) Potential well contour and profile in XZ dimension; b) potential well contour and profile in YZ plane

a)

b)

Figure 3.

a) Ion transmission vs. m/z plot showing the effective m/z range (inset shows 100% transmission of m/z 922) b) SLIM “elbow” structure (top panel) showing 90° turn of ions and SLIM “Tee” structure (bottom) to switch selected mobilities into orthogonal channel.

a)

b)

Figure 4.

a) Normalized potential profiles at different guard biases (central electrode length 10 mm) showing the structure and relative depth of the trapping well; b) contours of pseudo-potential well for the central rung electrodes of 6 mm (top panel) and 3 mm (bottom panel) length.

a)

b)

Figure 5.

a) Simulated and theoretical drift times through single SLIM straight component with path length 7.3 cm; b) experimental and predicted conditional resolving power after ion passage through six such SLIM straight components combined to constitute a 63.2 cm drift length.