Simulation Driven Design and Development of Structures for Lossless Ion Manipulations

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Overview

- "Pan-omics" MS-based measurements benefit greatly from IMS separations.
- IMS resolving power is limited by applied electric field and length of drift region.

$$R_{diffusion\ limited} = \frac{t}{\Delta t} = \sqrt{\frac{LEq}{16kBT\ln 2}}$$

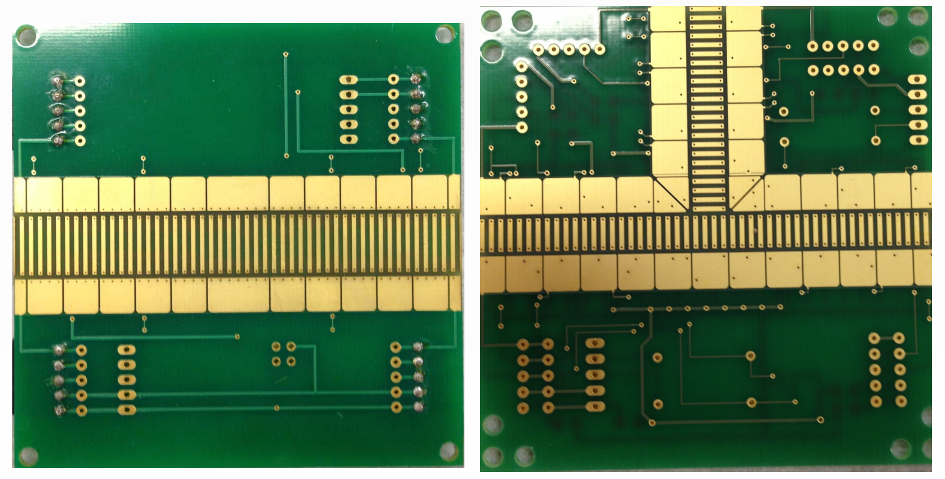
$$R_{gate\ limited} = \frac{t}{t_{gate}}$$

$$R^{-2} = (R_{diffusion\ limited})^{-2} + (R_{gate\ limited})^{-2}$$

- FAIMS, DMS, TW, Cyclotron devices are examples of systems that attempt at gas phase ion processing to improve or alter mobility resolving power.[1,2,3]
- However, previously developed devices have been incurred significant ion losses
- Ion manipulation devices that can provide platform for lossless, extended, complex gas phase ion manipulation are very attractive (SLIM devices).
- Theoretical/Computational evaluation of the devices is presented.

Introduction

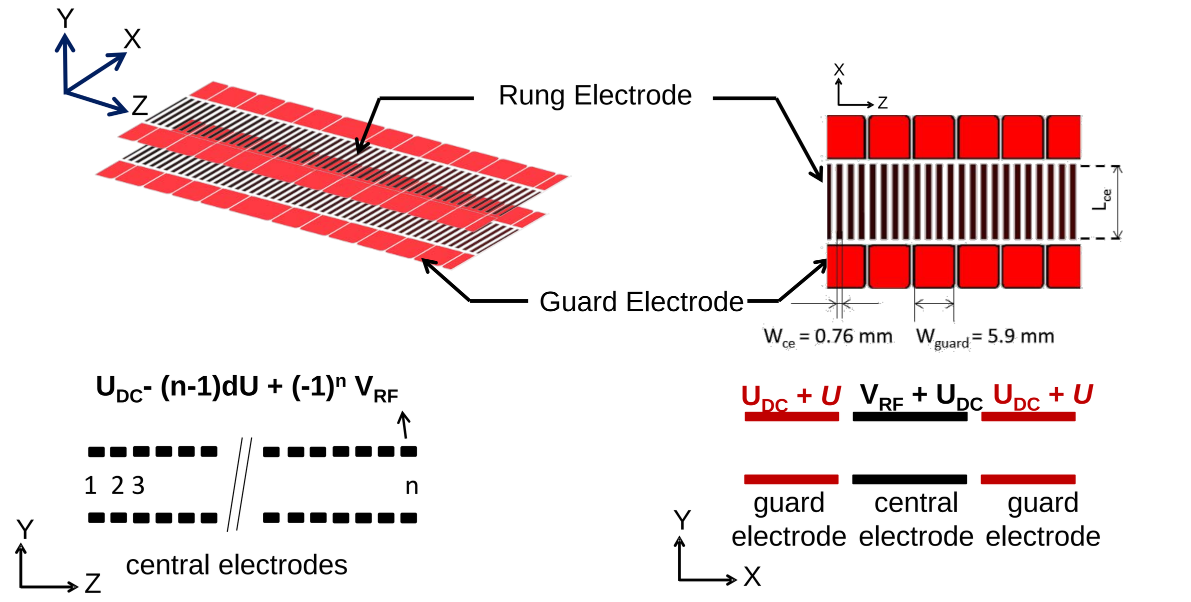
- Using printed circuit board technology planar devices for efficient ion trapping and drift have been constructed



- Straight, Tee, Elbow form the basic units which can be assembled to make devices for complex ion manipulation.
- Systematic studies of potentials and ion motion characteristics in these devices are essential for proof-of-concept, design, development and implementation.

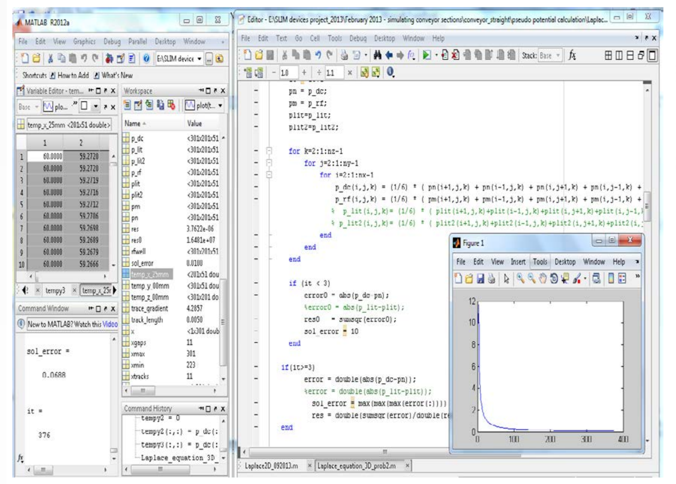
Methods

- Initial designs have 0.75 mm central electrodes with adjacent electrodes of opposite polarity superimposed with a DC gradient.
- Central electrodes are flanked by guard electrodes that provide confinement in XY plane using a DC bias
- Two planes of parallel electrodes are assembled together for trapping and manipulating ions.



- Simulation methods have been applied to these geometries to elucidate the device performance in terms of potentials and ion trajectories

Potential Well Depth Calculations

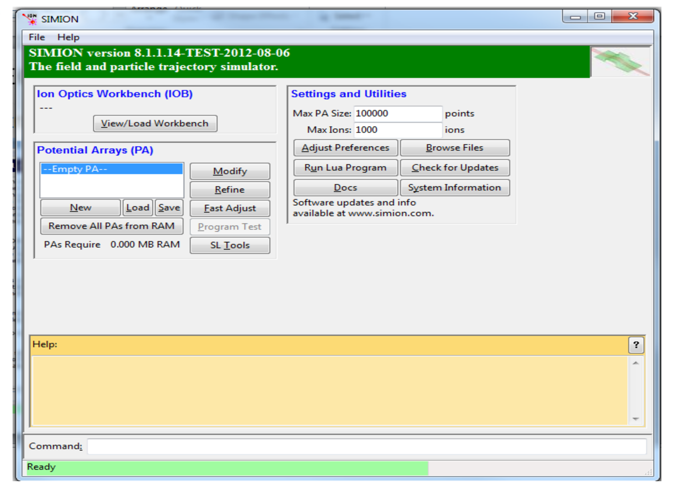


$$\varphi = \frac{q}{4m}\frac{|\nabla \phi_{RF}|^2}{\omega^2} + \phi_{DC}$$

$$\Delta\phi = 0$$

- Solving the pseudo-potential well depth.
- Finite Difference Method for numerical solution.
- Matlab implementation.

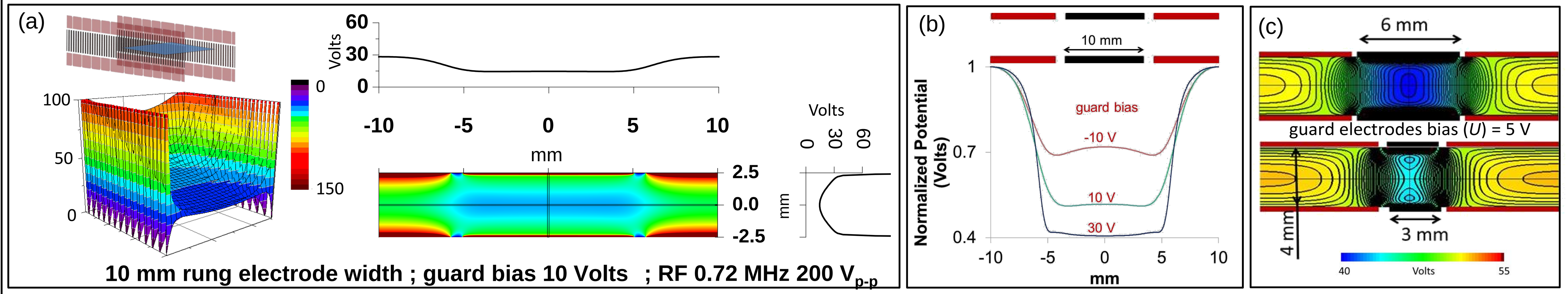
Ion Trajectory Simulations



- CAD designs were imported into SIMION 8.1.
- SDS collisions model for ion-neutral interaction.
- SIMION user codes for applying RF and DC potentials.

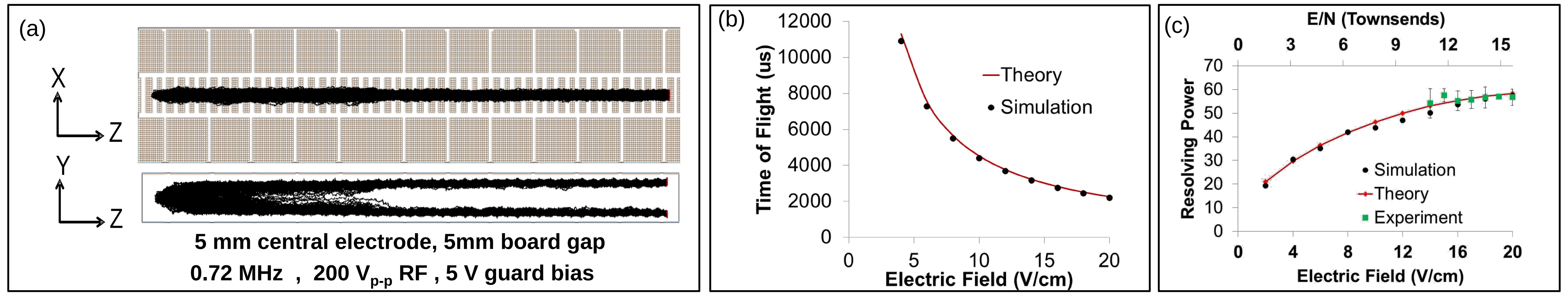
Results

1. Pseudo-Potential Well and Effects of Voltage and Geometry



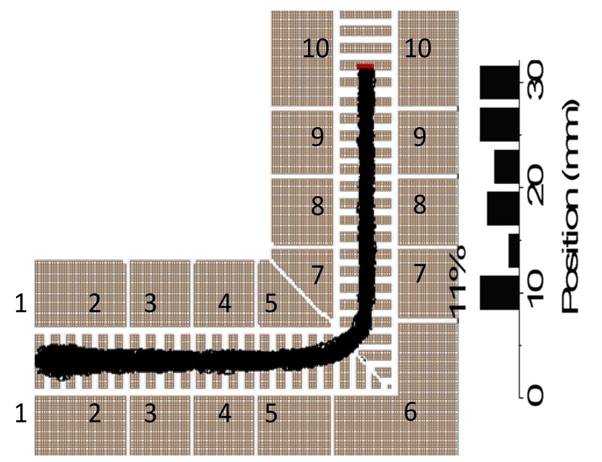
(a) Pseudo-potential well in the XZ and XY planes. (b) Trapping well profiles at different guard bias voltages. (c) Pseudo-potential well at different rung electrode widths

2. Lossless Ion Transport and Mobility Separations Using SLIM Devices



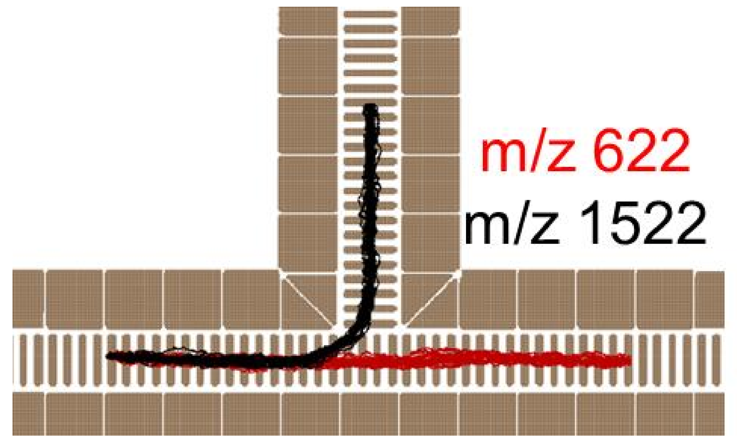
(a) Ion trajectories calculated by SIMION in a single straight SLIM unit. (b) Simulated and theoretical mean arrival time (m/z 1222) through a single SLIM unit. (c) Calculated, theoretical and experimental resolving power through 6 SLIM units (63.2cm long)

3. Lossless and Complex Manipulations of Ions in SLIM Devices



Transmission = 48%	Transmission = 100%
$V_7 = V_5 - 1^*\left[\frac{dV}{dn}\right]_{guard}$	$V_7 = V_5 - 3^*\left[\frac{dV}{dn}\right]_{guard}$
$V_6 = V_5 - 0.5^*\left[\frac{dV}{dn}\right]_{guard}$	$V_6 = V_5 - 1^*\left[\frac{dV}{dn}\right]_{guard}$

Voltage optimization is essential to execute a 90º turn. Simulation directed characterization of performance of turns achieved 100% transmission in simulations, which was replicated in experiments. Simulations were used to refine designs.



Switch Configuration	Transmission Efficiency(%)	Switch Efficiency (%)	Resolving Power
Normal straight	100	-NA-	13.1
Normal switch	99.9	100	12.1
Longer switch electrode (the orthogonal electrode at the junction is elongated)	90.8	100	13.1
Longer switch electrode and Insert electrode (elongated junction electrode and an additional insert electrode)	75	100	12.1

Simulations show a selected ion mobility (m/z 1522) was dynamically switched into an orthogonal SLIM channel The same polarity electrodes in the Tee inter-section contributed to loss of pseudo-potential and thereby loss of ions to electrodes. ~8% loss of resolving power is seen against comparable straight section due to race track effect. These losses was recovered through design iterations.

Conclusions

- Ion modeling/simulations have guided initial SLIM design, and subsequent refinements
- Close agreement of simulations with experiment give confidence in models for simulation-driven design
- Geometries and voltages can be used appropriately for manipulating ions in specific regions to expand applications to more complex manipulations

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