Study of Ion Confinement, Transport and Heating Effects in Traveling Wave Devices

Sandilya V.B. Garimella, Yehia M. Ibrahim, Roza Wojcik, Ian K. Webb, Richard D. Smith

Pacific Northwest NATIONAL LABORATORY

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Overview

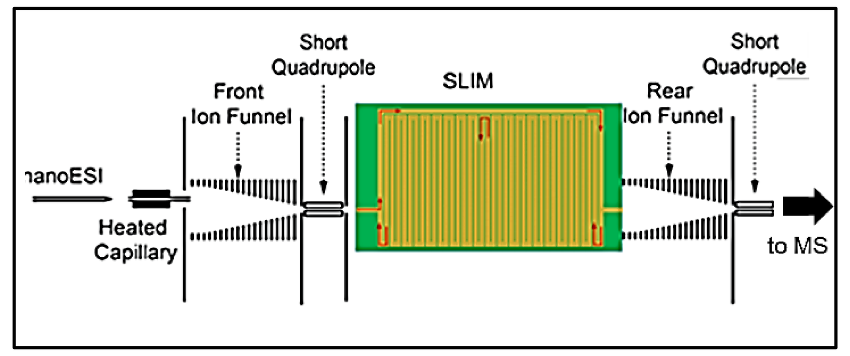
- Traveling Wave (TW) based ion mobility (IM) combined with mass spectrometry (MS) is being increasingly adopted for biological analysis
- Confinement and separations of ion structurers in TW-SLIM devices have been extensively studied[1,2]
- Biological applications benefit from gentle ion transport with minimal ion heating effects
- Herein we present a study of relative ion heating effects in TW devices through computations and experiments

Introduction

- Traveling wave ion guides provide IMS separations, but the relative heating effects under different configurations are not characterized.
- SLIM experimental parameters (geometry, electric fields) were varied to study relative heating effects on specific thermometer molecules (example Substance P).
- Ion effective temperature were calculated based on ion kinetic energies extracted from SIMION.
- A SIMION model was used to calculate the extent of ion population that changed confirmation due to the effective temperature
- Heating effects of a square traveling wave and AC wave have been compared experimentally and computationally.
- Different ion guide geometries are studied and characterized

Methods

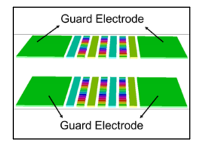
- **Experimental Setup:**



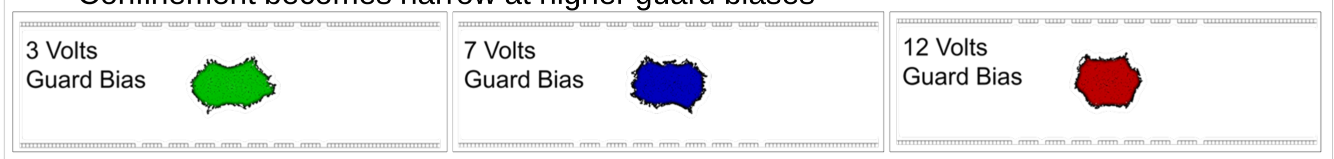
13 m SLIM board
4 RF strips , 3 TW path length : 1m
Square TW profile and AC sine Wave profile used for separations

- **Computational Models:**

Study of ion trajectories in SIMION 8.1:



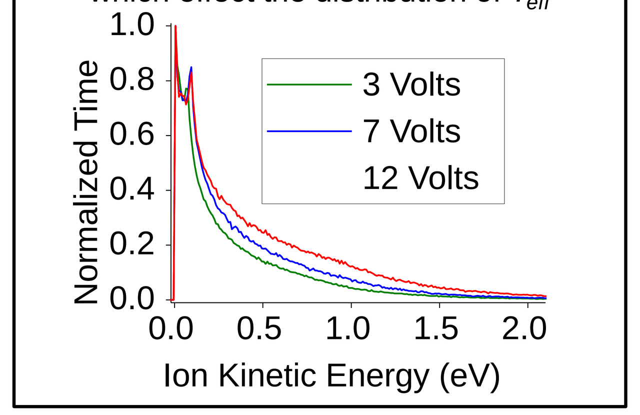
Confinement becomes narrow at higher guard biases



Ion Kinetic Energies and Ion Temperatures[3]**:** (at 2.5 torr)

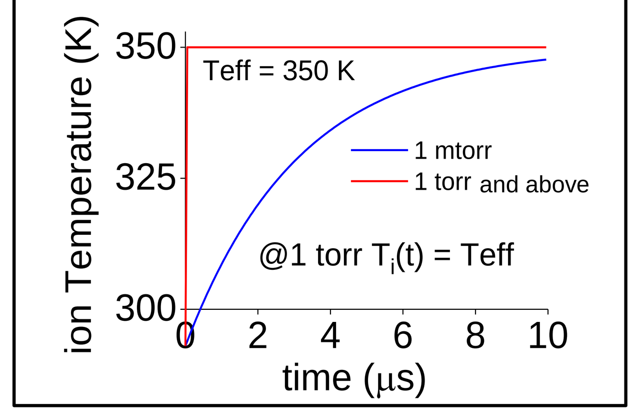
$$T_{eff} = \frac{m_r}{m_g}T + \frac{m_r}{m_g}\frac{2\langle K_i\rangle}{3\,k_B} \qquad \frac{dT_i}{dt} \approx \frac{(T_{eff} - T_i)}{\tau_h}$$

Ion Kinetic Energy (K_i) distributions (SIMION simulations in SLIM at 2.5 torr) can be modulated with applied voltages, which effect the distribution of T_{eff}



K_i changes with applied voltages

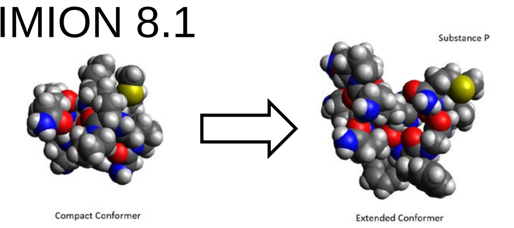
Time for ion to reach an equilibrium temperature is instantaneous at 2.5 torr



$T_i(t) = T_{eff}(K_i)$ at low E/N

Modeling Ion Structural Changes during Gas Phase Transport in Devices: The T_{eff} determines the ion structure. The evolution of ion trajectories of Substance P and the potential for unfolding due to TW and RF fields were modeled in SIMION 8.1

$$n_p = n_o\left[e^{-\left[\int_0^t Ae^{-\frac{E_a}{k_B\,T_{eff}(K_i)}}dt\right]}\right]$$



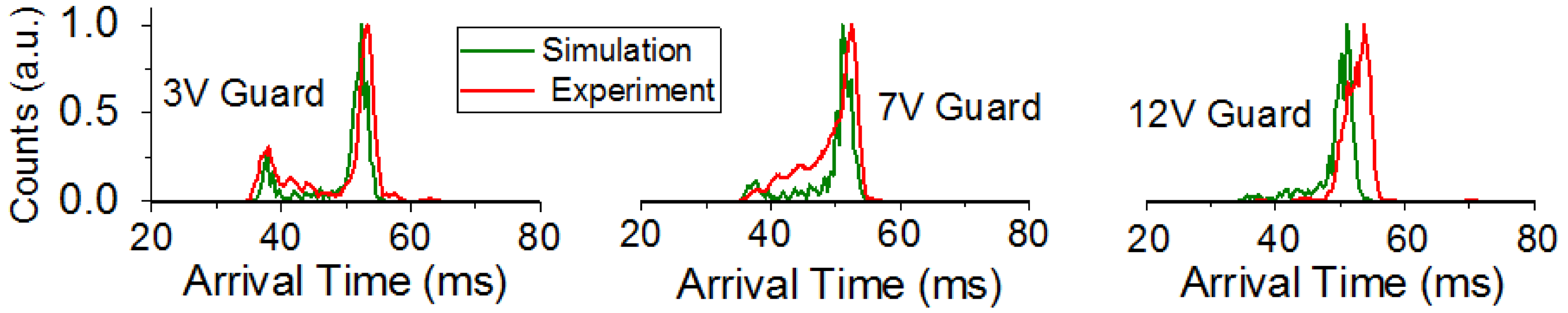
n_p – concentration of unfolded conformer n_o – concentration of folded conformer
E_a - Activation energy , A – Pre-exponential factor

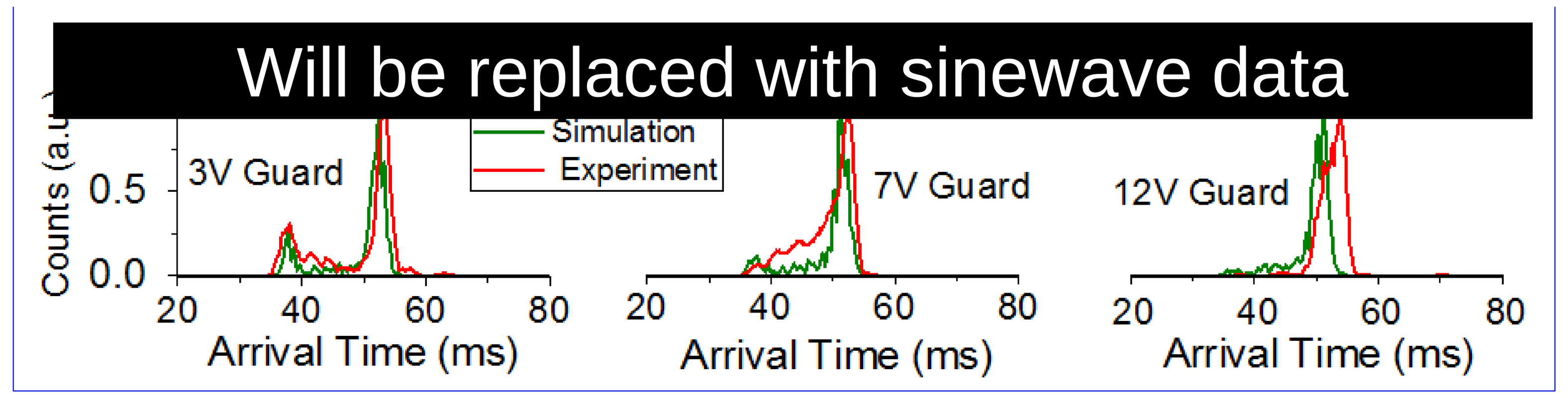
Results

Square Wave and Sine Wave in SLIM

Arrhenius Parameters: A = 6.3×10^{11} (1/s) E_a = 3.2 (eV)
Initial Population Distribution: 30% compact and 70% unfolded conformer

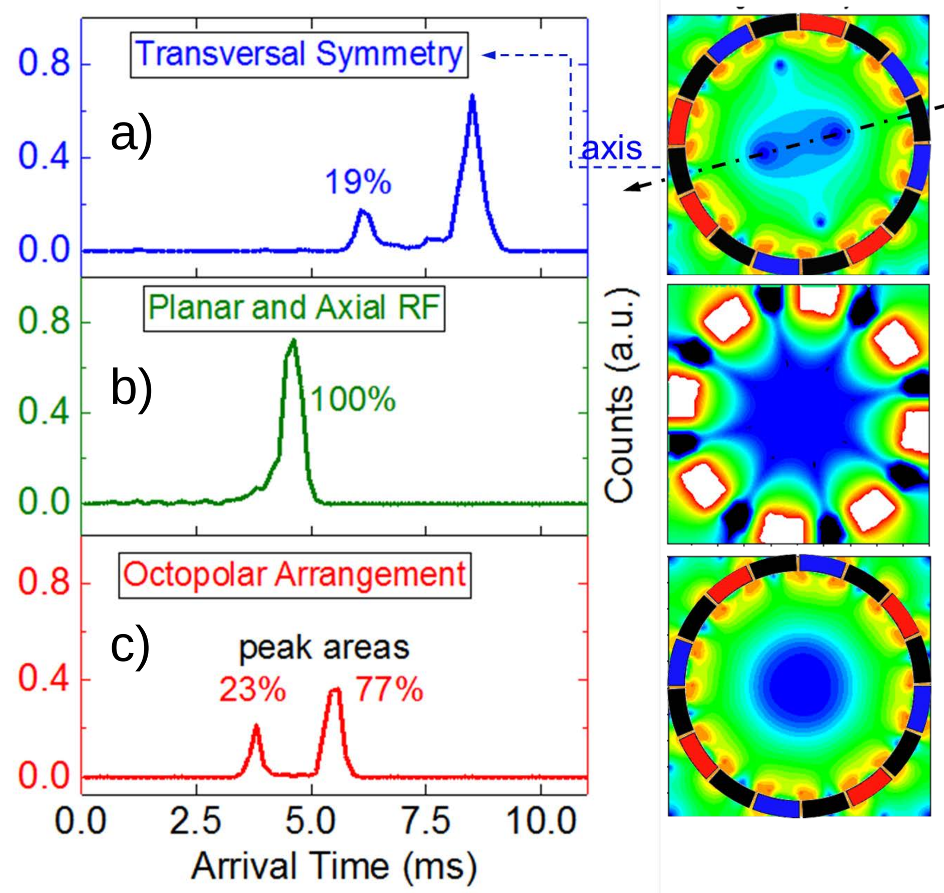
RF: 300 V_{pp} , 1 MHz Square TW: 20 V_{pp} , 60 kHz





Comparison of Different Circular Ion Guides

Initial Population Distribution: 25% compact and 75% unfolded conformer



The cross-section is symmetric about the axis (similar to a circularly arranged SLIM device)
The electric fields provide gentle confinement and transport as evidenced from 19% surviving compact conformer

Axial confinement (i.e. adjacent electrode rings have RF with opposite polarity in addition to opposite polarity within a segmented ring structure) results in excessive ion heating

Octopolar confinement is gentle and no ion activation is seen

Geometry "a" on the left has been adapted into a planar version in SLIM devices. Geometry "c" has been adapted into planar SLIM for dual polarity confinement and separations (see poster #Kwame)

Future and Conclusions

- A computational model that tracks evolving ion temperature (and ion structure) as it flies through an ion transport device operating at a few torr pressure has been built and validated.
- The model has been applied to study the relative heating effects during operation of SLIM
- AC waveforms have been found to be gentler than square waveforms
- Computational model of ion heating was used to study different arrangements of electrodes in circular conduits.
- A quadrupolar/Octopolar shape to the confinement potential provided practically no ion heating. Ion confinement with trapping RF in the direction of ion motion was found to be harsh in terms of ion heating.

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References

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Career Opportunities: For potential openings in Integrative Omics Group at PNNL please visit http://omics.pnl.gov/careers

CONTACT: Sandilya Garimella, Ph.D.
Biological Sciences Division
Pacific Northwest National Laboratory
E-mail: Sandilya.garimella@pnnl.gov

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