

# ASMS 2011 Posters/Sessions Related to SIMION

Poster: MP03 - Ion Mobility: Instrumentation and Fundamentals, poster number: 050, Monday, Poster Hall. **An Electrospray Ionization-Ion Mobility-Mass Spectrometer with Modular Periodic-Focusing DC Ion Guide.** Junho Jeon; Ryan Blase; Chaminda M. Gamage; David H. Russell. *Texas A&M University, College Station, TX*

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 086, Monday, Poster Hall. **Magnetic Field Inhomogeneity: Measurement, Consequences, and Compensation for Improved FT-ICR Mass Measurement.** Joshua Savory<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Brian Ruddy<sup>1</sup>; Steve Beu<sup>2</sup>; John Paul Quinn<sup>1</sup>; Chris Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>. <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*S C Beu Consulting, Austin, TX*

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 088, Monday, Poster Hall. **Characterization of Post-Injection Ion Kinetic Energy and Spatial Distribution in External Source FT-ICR MS.** Steve Beu<sup>1</sup>; Joshua Savory<sup>2</sup>; Nathan Kaiser<sup>2</sup>; Chris Hendrickson<sup>2</sup>; Alan G. Marshall<sup>3</sup>. <sup>1</sup>*S C Beu Consulting, Austin, TX*; <sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>3</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL*.

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 094, Monday, Poster Hall. **Evaluation Of Frequency Shifts In Particle-In-Cell Ion Trajectory Simulations Of Harmonized FT-ICR MS Analyzer Cells.** Franklin E. Leach III<sup>1</sup>; Andriy Kharchenko; Gleb Vladimirov<sup>3</sup>; Konstantin Aizikov; Peter B. O'connor<sup>5</sup>; Eugene Nikolaev<sup>3</sup>; Ron M.A. Heeren<sup>2</sup>; I. Jonathan Amster<sup>1</sup>. <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*FOM Institute for Atomic and Molecular Physics, Amsterdam, NETHERLANDS*; <sup>3</sup>*The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION*; <sup>4</sup>*BUSM, Boston, MA*; <sup>5</sup>*University of Warwick, Coventry, UNITED KINGDOM*

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 097, Monday, Poster Hall. **New method of ion beam shaping for increased sensitivity and performance stability of TOF MS.** James Bertsch; Michael Ugarov. *Agilent Technologies, Santa Clara, CA*

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 102, Monday, Poster Hall. **Ion cloud stabilization via ion-ion interactions in an ICR cell with inhomogeneous magnetic and inharmonic electric fields.** Gleb Vladimirov<sup>1</sup>; Yury Kostyukevich<sup>1</sup>; Christopher L. Hendrickson<sup>3</sup>; Greg T. Blakney<sup>4</sup>; Alan G. Marshall<sup>2</sup>; Eugene Nikolaev<sup>1,5</sup>. <sup>1</sup>*The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION*; <sup>2</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL*; <sup>3</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>4</sup>*National ICR Program at NHMFL, Tallahassee, FL*; <sup>5</sup>*The Institute of biochemical physics RAS, Moscow, Russian federation*

Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 104, Monday, Poster Hall. **Spectra of harmonics in the new dynamically harmonized FTICR cell.** Ivan Boldin<sup>1</sup>; Roland Jertz<sup>3</sup>; M Gokhan Baykut<sup>3</sup>; Eugene Nikolaev<sup>1,2</sup>. <sup>1</sup>*The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION*; <sup>2</sup>*The Institute of biochemical physics RAS, Moscow, RUSSIAN FEDERATION*; <sup>3</sup>*Bruker Daltonics, Bremen, Germany*

Poster: TP04 - New Developments in Ionization II, poster number: 067, Tuesday, Poster Hall. **Numerical Simulation of the Distribution of Ion Acceptance (DIA) in a commercial API Source.** Walter Wissdorf; Matthias Lorenz; Thorsten Benter. *University of Wuppertal, Wuppertal, GERMANY*.

Poster: TP04 - New Developments in Ionization II, poster number: 069, Tuesday, Poster Hall. **Computational Fluid Dynamic Model of a commercial Atmospheric Pressure Ion Source.** Thorsten Poehler<sup>2</sup>; Robert Kunte<sup>2</sup>; Herwart Hoenen<sup>2</sup>; Peter Jeschke<sup>2</sup>; Walter Wissdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>. <sup>1</sup>*University of Wuppertal, Wuppertal, GERMANY*; <sup>2</sup>*RWTH Aachen, Aachen, Germany*.

Poster: TP04 - New Developments in Ionization II, poster number: 070, Tuesday, Poster Hall. **Comparison and Validation of Atmospheric Pressure Ion Migration Models - Finite Elements Method vs. Discrete Particle Tracing.** Klaus J. Brockmann; Walter Wissdorf; David Mueller; Sonja Klee; Valerie Derpmann; Sebastian Klopotoski; Thorsten Benter. *University of Wuppertal, Wuppertal, GERMANY*

Poster: TP04 - New Developments in Ionization II, poster number: 075, Tuesday, Poster Hall. **Simulation of Ion movement in a 'long' gas dynamic interface.** Andrew Entwistle<sup>1</sup>; Alina Andreyeva<sup>2</sup>; Sergey Bulovich<sup>3</sup>; Mikhail Lapushkin<sup>5</sup>; Alexander Bazhenov<sup>4</sup>; Roger Giles<sup>1</sup>; Nicolay Gall<sup>5</sup>. <sup>1</sup>*Shimadzu Research Laboratory, Manchester, UK*; <sup>2</sup>*Institute for Analytical Instrumentation, Saint-Petersburg, RU*; <sup>3</sup>*S.-Petersburg State Polytechnical University, Saint-Petersburg, RU*; <sup>4</sup>*VNIIOkeangeology Institute, Saint-Petersburg, RU*; <sup>5</sup>*Physico-Technical Institute, Saint-Petersburg, RU*

Oral: WOC pm - Fundamentals: Ion-Surface Interactions and Preparative MS, time: 3:50, Wednesday, Room 401. **The Study of Ion Transmission and Soft Landing of Macromolecules Using Multiple Quadrupoles Instrument Coupled with MALDI Ion Source.** Ting-Chang Ko; Yao-Hsin Tseng; Wen-Ping Peng *National Dong Hwa University, Shoufeng, Hualien, TAIWAN*.

Oral: WOE pm - Instrumentation: New Developments in Instrumentation, time: 3:30, Wednesday, Korbel Ballroom 3-4. **Incorporation of Surface Induced Dissociation into an Ion Mobility – QTOF Mass Spectrometer for Post-Ion Mobility Activation.** Mowei Zhou<sup>1</sup>; Chengsi Huang<sup>1</sup>; Kevin Giles<sup>2</sup>; Anne Blackwell<sup>1</sup>; Vicki Wysocki<sup>1</sup>. <sup>1</sup>*University of Arizona, Tucson, AZ*; <sup>2</sup>*Waters Corporation, Manchester, United Kingdom*

Oral: WOE pm - Instrumentation: New Developments in Instrumentation, time: 3:50, Wednesday, Korbel Ballroom 3-4. **Design and Simulation of a Miniaturized Zaifman Trap for Electrostatic Storage of Ions with < 1 keV of Energy.** Ryan T. Hilger; Robert E. Santini; Scott A. Mcluckey. *Purdue University, West Lafayette, IN*.

Poster: ThP02 - Instrumentation: General, poster number: 020, Thursday, Poster Hall. **A new numerical code for calculation of electric field and simulation of ion motion in FT-ICR with arbitrary electrode geometry.** [Alexander Misharin](#)<sup>1</sup>; Alexander Popov<sup>2</sup>. <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>MSU, Moscow, Russia.

Poster: ThP02 - Instrumentation: General, poster number: 022, Thursday, Poster Hall. **Development of a Periodic-focusing DC Ion Funnel and Accumulation Device for an Electrospray Ionization Source.** [Kyle L. Fort](#); Joshua A. Silveira; David H. Russell. Texas A&M University, College Station, TX.

Poster: ThP02 - Instrumentation: General, poster number: 023, Thursday, Poster Hall. **Dynamics Simulation of Larger Molecules; Differential Mobility Analyzer with Newly Designed Mass Spectrometer Inlet.** Yi She; [Chenxi Zhu](#); Eiko Koizumi; Hideya Koizumi. Arkansas State University, State University, AR.

Poster: ThP02 - Instrumentation: General, poster number: 024, Thursday, Poster Hall. **High Dynamic Range Ion Detection Using Channel Electron Multipliers.** [Paul Mitchell](#); Stephen Ritzau; Lenny Erickson. Photonis USA, Inc., Sturbridge, MA.

Poster: ThP02 - Instrumentation: General, poster number: 026, Thursday, Poster Hall. **Computer Simulation of Ion Trajectories in Atmospheric Pressure Electrospray Ionization (AP-ESI).** [Kenichiro Saito](#)<sup>1</sup>; Yury Dessiaterik<sup>2</sup>; Eiko Koizumi<sup>1</sup>; Hideya Koizumi<sup>1</sup>. <sup>1</sup>Arkansas State University, State University, AR; <sup>2</sup>Colorado State University, Fort Collins, CO.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 042, Thursday, Poster Hall. **A Periodic-focusing DC Ion Funnel Interface for a Variable-temperature Ion Mobility Spectrometer.** [Joshua A. Silveira](#); Chaminda M. Gamage; David H. Russell. Texas A&M University, College Station, TX.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 044, Thursday, Poster Hall. **Considerations for the Design of an 8-Channel Spatially Multiplexed Ion Mobility-Mass Spectrometer.** [Jody May](#); Sevugarajan Sundarapandian; Kyle Osborne; John A. Mclean. Vanderbilt University, Nashville, TN.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 045, Thursday, Poster Hall. **Development of a Helical Dipole-based Atmospheric Interface Setup for Enhanced Ion Transfer Efficiency.** [Tamas Majoros](#)<sup>1</sup>; Daniel Szalay<sup>2</sup>; Gyorgy Hars<sup>3</sup>; Zoltan Takats<sup>4</sup>. <sup>1</sup>Semmelweis University, Budapest, HUNGARY; <sup>2</sup>Medimass Ltd., Budapest, Hungary; <sup>3</sup>Budapest University of Technology and Economics, Budapest, Hungary; <sup>4</sup>Justus-Liebig-University, Giessen, GERMANY.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 054, Thursday, Poster Hall. **FTIR Experiments on Mass Selected Cations by Counter-Ion Introduction Into an Inert Argon Matrix.** [Nathan Roehr](#); Jan Szczepanski; Nicolas Polfer. University of Florida, Gainesville, FL.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 061, Thursday, Poster Hall. **New Ion Trap Designs Obtained from Mapping Stability Diagrams and Determining Secular Frequency of Ion Oscillation Using Simion®.** [Joe Oliphant](#); Edgar Lee; Steve Lammert. Torion Technologies, Inc, American Fork, UT.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 063, Thursday, Poster Hall. **Transfer efficiency and timing performance measurements of multipole ion guides and ion wave guides constructed with planar technologies.** [Albrecht Glasmachers](#)<sup>1</sup>; Alexander Laue<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>; Michel Aliman<sup>2</sup>. <sup>1</sup>University of Wuppertal, Wuppertal, GERMANY; <sup>2</sup>Carl Zeiss NTS GmbH, Oberkochen, GERMANY.

Poster: ThP03 - Instrumentation: New Concepts, poster number: 064, Thursday, Poster Hall. **IonCCD™ for non-scanning sector-field instrument: from keV ion to image charge detection -- artifacts, performance and potential keV impact damage.** [Omar Hadjar](#)<sup>1</sup>; Thomas Schlathoelter<sup>2</sup>; Stephen Davila<sup>3</sup>; Gottfried Kibelka<sup>1</sup>; Scott Kassan<sup>1</sup>; Chad Cameron<sup>1</sup>; Ken Kuhn<sup>1</sup>; Guido F. Verbeck<sup>3</sup>. <sup>1</sup>ITT | OI Analytical, Pelham, AL; <sup>2</sup>KVI - Atomic and Molecular Physics, Groningen, The Netherlands; <sup>3</sup>University of North Texas, Denton, TX.

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 072, Thursday, Poster Hall. **Design of a Delayed Ion Injection Device to Improve the Detection Mass Range and the Sensitivity of FT-ICR MS.** [Myoung Choul Choi](#); Kyu Hwan Park; Hyun Sik Kim. Korea Basic Science Institute, Ochang-Myun, SOUTH KOREA.

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 075, Thursday, Poster Hall. **Development of a portable mass spectrometer for operation at 1 Torr.** [Feng Jin](#)<sup>1</sup>; Guido F. Verbeck<sup>2</sup>; Glen P. Jackson<sup>1</sup>. <sup>1</sup>Ohio University, Athens, OH; <sup>2</sup>University of North Texas, Denton, TX

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 078, Thursday, Poster Hall. **Metrological characterization of a sensitive secondary ion mass spectrometer for electron microscopes to combine optical/structural and analytical imaging.** [Alexander Laue](#)<sup>1</sup>; Albrecht Glasmachers<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>; Michel Aliman<sup>2</sup>; Hubert Mantz<sup>2</sup>. <sup>1</sup>University of Wuppertal, Wuppertal, GERMANY; <sup>2</sup>Carl Zeiss NTS GmbH, Oberkochen, GERMANY

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 083, Thursday, Poster Hall. **Lenses or No Lenses? A Study of Ion Transfer Efficiency at Interfaces in a Lens-less Triple Quadrupole MS.** [Felician Muntean](#); Roy Moeller. Bruker Daltonics, Walnut Creek, CA.

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 086, Thursday, Poster Hall. **Ion trajectory calculations of ions entrained in neutral gas flow in the quadrupole field, utilizing superimposed flow fields and electric fields.** [Serguei Savtchenko](#)<sup>1</sup>; [Evgeny Makeev](#)<sup>1</sup>; Jean-Francois Alary<sup>2</sup>; Sha Joshua Ye<sup>1</sup>. <sup>1</sup>IONICS Mass Spec Group, Inc., Bolton, ON; <sup>2</sup>Isobarex Corp., Bolton, ON.

Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 087, Thursday, Poster Hall. **Significant Improvements in Trapping Efficiency of Externally Injected Ions Using a Cylindrical Ion Trap with Increased Buffer Gas Pressure.** [Michael Goodwin](#); Mitch Wells. FLIR Mass Spectrometry (Griffin), West Lafayette IN, 47906.

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Poster: MP03 - Ion Mobility: Instrumentation and Fundamentals, poster number: 050, Monday, Poster Hall

### **An Electrospray Ionization-Ion Mobility-Mass Spectrometer with Modular Periodic-Focusing DC Ion Guide**

Junho Jeon; Ryan Blase ; Chaminda M. Gamage; David H. Russell  
*Texas A&M University, College Station, TX*

**Novel Aspect:** An ESI-IF interface coupled to a modular PDC IG for high resolution and high sensitivity ion-mobility mass spectrometry is described

#### **Introduction**

Increasing the transmission and resolution of ion mobility spectrometry (IMS) is essential for increasing chemical/biological applications. We have developed periodic-focusing DC ion guide (PDC IG) providing increased transmission and minimal loss in resolution based on electrode geometry and we have coupled these devices to a novel modular PDC IG IM-MS apparatus. This instrument is equipped with an RF ion funnel (IF) home-built electrospray ionization time-of-flight mass spectrometer (ESI-TOF MS) to achieve higher transmission of ions leading to better sensitivity with less resolution detriment. The design and optimization of the system in terms of hybridization with three distinctive ion transmission regions (IF-PDC IG-TOF) will be discussed.

#### **Methods**

A conventional (rf) ESI-IF consisting of 34-lens elements with a 2 mm exit aperture and PDC IG optimized using SIMION® 8.0 has been interfaced to a home-built IM-MS instrument. Ions exiting the IF enter a modular PDC IG IM drift cell; drift cell length is 23 cm (composed of 17 electrodes) with a thickness: spacing: inner diameter ratio of 6 mm: 6 mm: 8 mm and an exit orifice of 800  $\mu\text{m}$ . Coupling of additional modules can extend the ion mobility spectrometer length. The PDC IG is interfaced to a linear orthogonal TOF using four periodic electrodes (as ion guides) and Einzel lens. The mass spectra obtained from sample solutions are recorded using Ionwerks® 2-D data acquisition software.

#### **Preliminary Data**

The radial RF and axial DC potentials of the ESI-IF ion provide efficient ion transport from atmosphere to the differentially pumped region separating the ion source and ion mobility drift cell, which is maintained at  $\sim 0.5$  to  $\sim 1.5$  torr. For example, a 25  $\mu\text{M}$  solution of bradykinin (1-8) provides ion currents of up to 15 nA using standard focusing conditions; 70Vpp at 800 kHz RF and 10V/cm DC and pressures of 0.8 torr, and simulated (assuming static pressure) ion trajectories (assuming hard sphere collisions) suggests that ion transmission of  $>90\%$  are achievable. The interface between the ESI-IF and the ion mobility drift cell is critical to optimum performance of the instrument. That is, this region also provides differential pumping between the atmospheric pressure ESI ion source and operating pressure (1-5 torr) of the ion mobility drift cell. Of equal importance for accurate collision cross section measurements possible contamination of the IM drift gas from impurities, including residual ESI solution. Although rf ion-guides can be used in this region to achieve high ion transmission, for experimental simplicity we chose to use a PDC IG as the interface. Experiments that demonstrate the utility of PDC IG as an effective ion-guide for ESI-IM-MS will be presented. This presentation will provide detailed explanations of the theory of the PDC IG interface as well as experiments that support the predictions of the theory. In addition, data that support our prior claims that PDC IF drift cells can be used for higher transmission, high resolution and high sensitivity ion mobility will be presented.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 086, Monday, Poster Hall

### **Magnetic Field Inhomogeneity: Measurement, Consequences, and Compensation for Improved FT-ICR Mass Measurement**

Joshua Savory<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Brian Ruddy<sup>1</sup>; Steve Beu<sup>2</sup>; John Paul Quinn<sup>1</sup>; Chris Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>  
*<sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>S C Beu Consulting, Austin, TX*

**Novel Aspect:** An FT-ICR magnetic field gradient is measured and correlated with experimental and simulated observations.

#### **Introduction**

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) relies upon excitation and detection of ion cloud radial motion in superimposed spatially uniform static magnetic and linear electric fields. Ion cloud coherence determines the quality of the measurement (i.e., obtainable resolving power, S/N, etc.) and depends upon the spatial homogeneity of the magnetic field. Magnetic field inhomogeneity is intrinsic to magnet design and construction. Cryogenic and room temperature shims improve but don't perfect homogeneity. In this work, we use magnetic field measurements from a 9.4 tesla FT-ICR MS to improve simulation accuracy and to correlate observations from experiment and simulation.

#### **Methods**

**Magnetic Field Measurement.** Field measurements were recorded with and without the mass spectrometer positioned in the bore of our 9.4 tesla (Oxford Instruments) magnet by use of a custom probe mount. The axial field strength was measured with a Metrolab NMR Precision Teslameter at 26 locations on axis as well as 12 axial locations and 12 angular positions for radii of 20 mm and 37 mm.

**Simulations.** Computer simulations were performed in SIMION 8 with an ion image charge detection model (Hendrickson et al.; *International Journal of Mass Spectrometry* **2009**, 283(1-3), 100-104). A realistic magnetic field gradient was incorporated into the model by expansion of the axial field measurements to obtain the radial field gradients.

## Preliminary Data

Magnetic field measurements performed in the 9.4 Tesla magnet yield an approximately 11 ppm peak-to-peak variation in field strength over a cylindrical region 60 mm in length and 70 mm in diameter. Magnetic field inhomogeneity induced frequency shifts in all three modes of ion motion (cyclotron, magnetron, and axial) depend on  $m/z$ , ion axial amplitude, and radius (Mitchell et al.; *International Journal of Mass Spectrometry and Ion Processes* **1994**, 141, 101-116). Magnetic field inhomogeneity causes loss of ion signal at extended transient duration and systematic error in the frequency-to-mass conversion used to calibrate the measured frequency spectrum. Experimental measurements show that the optimal compensation electrode voltage for a 7-segment open cylindrical ICR cell (Tolmachev, A. V. et al.; *Journal of the American Society for Mass Spectrometry* **2008**, 19, 586-597) deviates from the most quadrupolar electric field, and depends on ion  $m/z$  and magnetic field gradient. We also compare the  $m/z$ -dependent systematic deviation from the two-term equation typically used for calibration to reduced cyclotron frequency determined from SIMION 8 as a function of ion axial amplitude,  $m/z$ , and radius with and without the addition of a realistic magnetic field gradient.

Supported by the NSF Division of Materials Research through DMR-0654118 and the State of Florida.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 088, Monday, Poster Hall

### Characterization of Post-Injection Ion Kinetic Energy and Spatial Distribution in External Source FT-ICR MS

Steve Beu<sup>1</sup>; Joshua Savory<sup>2</sup>; Nathan Kaiser<sup>2</sup>; Chris Hendrickson<sup>2</sup>; Alan G. Marshall<sup>3</sup>

<sup>1</sup>S C Beu Consulting, Austin, TX; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL

**Novel Aspect:** Computer simulations and experimental measurements characterize post-injection ion kinetic energy and spatial distribution in external source FT-ICR MS.

#### Introduction

Figures of merit for FT-ICR MS are significantly affected by ion initial kinetic energy and spatial distribution in the ICR cell because those distributions affect the extent to which ions experience electric and magnetic field inhomogeneities after excitation of cyclotron motion. Prior work has shown that excitation of radial motion and exchange of axial and radial energy can occur during injection of ions from an external source in a multipole ion guide (1,2). In this work we use computer simulations and experimental measurements to characterize the impact of those processes on post-injection ion kinetic energy and spatial distribution, and extend prior models to include initial ion trajectories that are not well focused on the axis of the multipole.

#### Methods

Simulations were performed with SIMION (Version 8.0, Scientific Instrument Services) running on a homebuilt 3.00 GHz AMD Phenom II Quad-Core PC with 8 GB DDR3 ram. Octopole and quadrupole ion guides with an inscribed radius of 2.38 mm were modeled with an array resolution of 0.0635 mm. Analytical descriptions of the three-dimensional magnetic field components of an existing 9.4 T magnet and the proposed 21 T magnet under development at the National High Magnetic Field Laboratory were incorporated in the simulations by means of SIMION user programs. Experimental determinations of ion kinetic energy and axial distribution were accomplished by application of retarding potentials and acquisition of time-of-flight profiles for a 9.4T FT-ICR MS.

## Preliminary Data

Prior modeling has shown that two principal effects alter ion kinetic energy during traversal of a strong magnetic field gradient in a multipole ion guide. The first is resonant acceleration of cyclotron motion that occurs when ions encounter a magnetic field at which the ion cyclotron frequency equals the multipole drive frequency divided by the multipole order. The second effect is an exchange of axial and radial ion kinetic energy caused by the axial force that results from ion motion perpendicular to the radial component of the magnetic field gradient. The force generally causes axial deceleration with concomitant increase in radial kinetic energy. The extent of transient resonance and axial deceleration vary with initial ion radial kinetic energy, and ion trajectories initially focused on the multipole axis result in narrow post-injection kinetic energy distribution for fixed initial radial energy. In this work we extend simulations to include the more general case of initial ion trajectories that are not directly focused on the axis upon entrance to the multipole, which reveals a significant broadening of the post-injection radial and axial ion kinetic energy distributions, and associated spatial distribution. The change in distribution is shown to correlate with the magnitude and orientation of an initial azimuthal velocity component (i.e., a component perpendicular to a plane containing the multipole axis) that is not present for trajectories initially focused on the multipole axis.

This work was supported by NSF Division of Materials Research through DMR-0654118 and the State of Florida.

[1] S. C. Beu, C. L. Hendrickson, and A.G. Marshall, *J. Am. Soc. Mass Spectrom.* 2011, 22, 000-000.

[2] S. C. Beu, C. L. Hendrickson, and A.G. Marshall, *Proc. 57th ASMS Conf. on Mass Spectrometry and Allied Topics*, Philadelphia, PA, 31 May - 4 June 2009. TPK279.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 094, Monday, Poster Hall

### Evaluation Of Frequency Shifts In Particle-In-Cell Ion Trajectory Simulations Of Harmonized FT-ICR MS Analyzer Cells

Franklin E. Leach III<sup>1</sup>; Andriy Kharchenko; Gleb Vladimirov<sup>3</sup>; Konstantin Aizikov; Peter B. O'connor<sup>5</sup>; Eugene Nikolaev<sup>3</sup>; Ron M.A. Heeren<sup>2</sup>; I. Jonathan Amster<sup>1</sup>

<sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>FOM Institute for Atomic and Molecular Physics, Amsterdam, NETHERLANDS; <sup>3</sup>The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION; <sup>4</sup>BUSM, Boston, MA; <sup>5</sup>University of Warwick, Coventry, UNITED KINGDOM

**Novel Aspect:** Application of multi-particle ion trajectory simulations to evaluate frequency shifts in harmonized FT-ICR mass analyzers

### Introduction

The design of enhanced mass analyzers remains topical within the Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) community as the need for increased experimental performance to solve complex chemical problems with the provision of ultra-high mass accuracy and resolving power persists. This performance is dependent upon the applied magnetic field as well as the electric potentials generated within the mass analyzer. As the applied trapping potential becomes more quadrupolar by harmonization of the field, excitation to higher cyclotron radii is possible, which reduces space charge effects while increasing image charge interactions. To examine these frequency shifts within harmonized mass analyzer designs, particle-in-cell (PIC) ion trajectory simulations and harmonic inversion by the filter diagonalization method (FDM) are employed.

### Methods

Multi-particle ion trajectory simulations were run remotely on a Linux cluster located at FOM-AMOLF. Mass analyzers of semi-arbitrary geometry were generated in SIMION 8.0 and electric fields calculated prior to using particle-in-cell methods to enable coulombic interactions during ion trajectory calculations. Ion populations were varied in ion number and m/z while constrained radially by a magnetic field and trapped axially by a harmonized potential. Ion excitation was modified to produce cyclotron orbits of varying radii. A time domain transient was acquired and a frequency domain spectrum was derived using the fast Fourier transform (FFT) as well as the filter diagonalization method (FDM).

### Preliminary Data

Prior experimental studies have demonstrated that the space charge induced frequency shift during FT-ICR MS image current detection can be reduced by excitation to higher cyclotron radii where ion densities decrease. Visualization of ion cloud motion from PIC ion trajectory calculations reveals a reduction in cloud density, in agreement with theory and prior experiment, but this action increases the image charge interaction. Building upon prior work, the cyclotron frequencies are determined by harmonic inversion of the simulated time domain transient by the filter diagonalization method (FDM) as the excitation radius is varied to induce a change in ion cloud density. Frequency calculations reveal a decrease in the instantaneous frequency shift due to attributed to space charge interaction on the order of Hz as the orbital radius is increased. Although this reduces space charge effects, ion cloud coherence is impaired by excitation into inhomogeneities of the trapping potential and limits the duration of the time domain signal.

Construction of mass analyzers in silico and subsequent field calculation via SIMION allows for the evaluation of the electric field gradient. Selected mass analyzer geometries for simulation employ aspects of harmonization, which allow for more ideal trapping potentials. One aspect of these improvements is that higher excitation radii can be achieved, minimizing the space charge interaction, while maintaining ion cloud coherence as electric field inhomogeneities are reduced. Comparisons of time domain signal coherence, ion cloud, and frequency shifts due to space charge and image charge interaction are compared amongst selected designs. To differentiate frequency shift contributions due to image charge, simulations of a single m/z population are conducted.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 097, Monday, Poster Hall

### **New method of ion beam shaping for increased sensitivity and performance stability of TOF MS**

James Bertsch; Michael Ugarov  
Agilent Technologies, Santa Clara, CA

**Novel Aspect:** Novel ion beam formation optics improves sensitivity and performance stability of TOF MS

### Introduction

Current high performance Time-of-flight (TOF) mass spectrometry is expected to offer the combination of high sensitivity, mass accuracy and resolution. Improvements in the source technology, as well as extension of the ion path inside the analyzer have been recently seen to promote TOF mass spectrometry to the position of being able to provide quantitation and high selectivity profiling simultaneously.

Still, there is one factor that remains critical for the high performance of this type of mass analyzers – the formation of a high quality ion beam before it enters the orthogonal extraction region. We report the new development of a novel ion optics design that achieves high resolution, high transmission and performance stability.

### Methods

Ion beam shaping optics (the “slicer”) of the Quadrupole TOF mass analyzer has been modified. This instrument relies on Ion Beam Compressor (IBC) technology which provides cooling and focusing of ions before they leave the cavity filled with collision cell gas. The new optics is expected to achieve improved performance based on the fact that the skimming of the ion beam is performed using one narrow slit which can be maintained at elevated potential with respect to the rest of the optics. Additional elements have been

added to the design of the slicer to achieve the optimum beam formation in two dimensions. This arrangement also allows easy tuning of the instruments performance parameters, such as resolution and sensitivity.

#### **Preliminary Data**

Various configurations of optics have been designed. Simion modeling was performed assuming the output distribution of ion velocities after the focusing in the IBC. The prototypes have been built and tested.

Preliminary results suggest that the formation of an ion beam with small cross section and divergence can be achieved when only one slit is used. The slicer has been operated with the slit maintained at high negative potential in order to achieve a high degree of ion acceleration. As a result, the performance is less sensitive to potential non-uniformities or contamination issues. Very high (100's of hours) operation longevity was demonstrated. Injection of very high amounts of analyte did not result in performance degradation that would require optics cleaning. This result was also facilitated by the use of special slit geometries that were employed to minimize the effect of contamination on the ion beam.

The optimized geometry of the ion optics allowed achieving good quality beam in two dimensions which is critical for maximizing the transmission, and therefore, the sensitivity of the analysis. Preliminary data suggest that not just the performance stability, but also the sensitivity of the instrument can be improved considerably (up to 100%) at no cost to mass resolution and mass accuracy.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 102, Monday, Poster Hall

#### **Ion cloud stabilization via ion-ion interactions in an ICR cell with inhomogeneous magnetic and inharmonic electric fields**

Gleb Vladimirov<sup>1</sup>; Yury Kostyukevich<sup>1</sup>; Christopher L. Hendrickson<sup>3</sup>; Greg T. Blakney<sup>4</sup>; Alan G. Marshall<sup>2</sup>; Eugene Nikolaev<sup>1,5</sup>

<sup>1</sup>The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION; <sup>2</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>3</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>4</sup>National ICR Program at NHMFL, Tallahassee, FL; <sup>5</sup>The Institute of biochemical physics RAS, Moscow, Russian federation

**Novel Aspect:** Explanation of ion cyclotron motion phase locking at high ion number in an FT-ICR cell

#### **Introduction**

Resolution in FT-ICR mass spectrometry is limited by the duration of spatially coherent ion cyclotron motion. In the absence of ion-neutral collisions, the two main sources of phase coherence loss are spatially inhomogeneous magnetic field and inharmonic electrostatic trapping potential, leading to "comet-like" ion cloud shape. However, such coherence loss may be alleviated by increasing the number of trapped ions, leading to ion cloud alignment ("ion condensation" or "phase locking" [1]). Here, we employ large-scale simulations to elucidate the mechanism of ion condensation.

#### **Methods**

Dynamics of ion cloud motion in an ICR cell were simulated by use of the Particle-In-Cell (PIC) algorithm [1] with the net electric field calculated via the trap potential approximation  $V=A(2z^2-r^2)+B_1 z^3+B_2 z^4+C_1 r^3+C_2 r^4$  and SIMION 8. The space charge electric field of for ion clouds was calculated by solving Poisson's equation. Inhomogeneous magnetic field was approximated by a binomial series expansion. All calculations were performed for ions of a single m/z.

#### **Preliminary Data**

Ion cloud condensation consisting of formation of compact elliptically shaped ion clouds after reaching a critical ion cloud population has been observed in [1]. Detailed characterization of that phenomenon reveals that: (1) the number of ions required for condensation is independent of magnetic field strength; and (2) for higher electrostatic and magnetic field imperfection, more ions are required to produce condensation. Detailed analysis of ion trajectories and velocities shows that ion condensation occurs due to changes in ion axial oscillation. After the number of ions in the cloud reaches a critical value, ion axial oscillation amplitudes become equal, making effective cyclotron frequencies in the whole ion ensemble equal and preventing comet formation. Work supported in part by the USA National Science Foundation (NSF) Division of Materials Research through DMR-06-54118 and the State of Florida.

1.Eugene N. Nikolaev, Ron M. A. Heeren, Alexander M. Popov, Alexander V. Pozdnev, Konstantin S. Chingin, Realistic modeling of ion cloud motion in a Fourier transform ion cyclotron resonance cell by use of a particle-in-cell approach Rapid Commun. Mass Spectrom. 2007; 21, 3527–35462.

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Poster: MP05 - High Mass Accuracy / High Performance MS: Instrumentation, poster number: 104, Monday, Poster Hall

#### **Spectra of harmonics in the new dynamically harmonized FTICR cell**

Ivan Boldin<sup>1</sup>; Roland Jertz<sup>3</sup>; M Gokhan Baykut<sup>3</sup>; Eugene Nikolaev<sup>1,2</sup>

<sup>1</sup>The Institute for Energy Problems of Chemical Phys, Moscow, RUSSIAN FEDERATION; <sup>2</sup>The Institute of biochemical physics RAS, Moscow, RUSSIAN FEDERATION; <sup>3</sup>Bruker Daltonics, Bremen, Germany

**Novel Aspect:** High-order odd and even harmonics in the new dynamically harmonized FTICR cell are obtained and analyzed

## Introduction

A new FTICR cell design based on the principle of dynamic harmonization of trapping field has been proposed by us recently [1]. The cell has excitation and detection electrodes of parabolic shape in order to form trapping electric field that is harmonic upon being averaged over a cyclotron period of an ion. This cell has already demonstrated the highest resolution ever achieved on 7 T magnets. However due to specific design of detection electrodes the spectrum of high-order harmonics should look different from what is observed on conventional FTICR cells. In this work we reveal the features of harmonics' spectra in our new FTICR cell.

## Methods

Compared to a conventional FTICR cell the current version of our dynamically harmonized cell has each of its detection electrodes split into three parts of complex shape. These three electrodes are connected within the cell to be included into a normal detection circuit. The signal generated by this configuration is expected to include harmonics of higher intensities than cylindrical or open cell. We have investigated the spectra of harmonics for the new cell both theoretically and experimentally. Experiments were done on 7 Tesla Bruker FT ICR instrument.

## Preliminary Data

Theoretical spectra of high-order harmonics were simulated using SIMION 8.0 with reciprocity principle used to calculate ion signal. Experimental data were collected using Bruker 7 T magnet. Experimentally obtained spectra of high-order harmonics contain up to 11-th harmonic. The intensities of harmonics in the new cell are compared to the open-type cell. The dependencies of harmonics' intensities on excitation amplitude are presented. They are compared to simulated dependencies in order to set up a correspondence between intensities of high-order harmonics (related to the signal intensity) and ion cyclotron radius. This correspondence shows that in our new FTICR cell cyclotron radius can reach up to 80% of cell inner radius.

[1] Boldin, I.A.; Nikolaev, E.N. FTICR cell with dynamic harmonization of the electric field in the whole volume by shaping of excitation and detection electrode assembly. *Rapid Commun Mass Spec* 2011, 25, 122-126.

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Poster: TP04 - New Developments in Ionization II, poster number: 067, Tuesday, Poster Hall

### Numerical Simulation of the Distribution of Ion Acceptance (DIA) in a commercial API Source

Walter Wissdorf; Matthias Lorenz; Thorsten Benter  
*University of Wuppertal, Wuppertal, GERMANY*

**Novel Aspect:** First successful numerical model for DIA simulations in a highly complex AP ion source geometry with experimental validation

## Introduction

The Distribution of Ion Acceptance (DIA) in AP ion sources depends on electrical and fluid dynamic forces and provides a direct but complex insight into the prevailing dynamical processes. The interpretation of DIA data needs to include the neutral analyte density distribution, gradients responsible for transport of ions and neutrals, as well as transformation processes, i.e., chemical change. It is thus of fundamental interest for deterministic AP ion source development to be able to model new approaches with some accuracy. A valid numerical model of these dynamical processes would open a gateway to a whole new design approach for AP ion optical devices, i.e., from trial and error towards model driven engineering.

## Methods

Computational Fluid Dynamic (CFD) simulations of a Bruker Multi Purpose Ion Source (MPIS) were performed with Ansys CFX 12.1. Ion trajectory simulations were performed with SIMION v.8.0 with the statistical diffusion simulation (SDS) extension using CFD results as input. For interfacing between the software packages and data interpretation a home-made software package was implemented using different programming languages (Python, Lua, Matlab). DIA measurements were performed in an MPIS connected to a Bruker micrOTOF mass spectrometer equipped with a laser ionization (APLI) source. The laser beam was spatially adjusted with a computer controlled optical stage. The recorded ion intensity as function of the ionization position is referred to as the "Distribution of Ion Acceptance".

## Preliminary Data

The numerical simulation of the distribution of ion acceptance (DIA) in a commercially available ion source requires a coupled i) validated fluid dynamical model, ii) the neutral analyte distribution, and iii) an ion migration model as basis. A validation of the *entire approach* is possible by comparing experimentally and numerically determined distributions of ion acceptance. Preliminary DIA simulation results on the basis of a limited set of CFD simulations clearly shows the feasibility of the present approach. The overall shape of experimentally determined DIA, as reported in the literature, was numerically reproduced and the dependence of *numerically derived DIA* on external parameters, i.e., electrical and fluid dynamical forces, are in very good agreement with *experimentally observed DIA* dependencies. The reasons for the formation of the complex DIA shapes both in the experiments as well as in the models are clearly identified as distinct features of the fluid flow and the neutral analyte distribution. With the performed simulations it was possible to identify critical regions of the gas inlet geometry of the ion source with respect to the overall performance. These were considered essentially non-critical during the experiments. These surprising findings show that a numerical model-driven development and optimization process of AP ion sources is possible. We will present a comprehensive overview of the performed DIA simulations, a comparison with experimentally derived DIA, and a critical discussion of the results. Further development of the outlined approach could lead to significant progress in computationally supported AP ion optical device optimizations.

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Poster: TP04 - New Developments in Ionization II, poster number: 069, Tuesday, Poster Hall

**Computational Fluid Dynamic Model of a commercial Atmospheric Pressure Ion Source**  
Thorsten Poehler<sup>2</sup>; Robert Kunte<sup>2</sup>; Herwart Hoenen<sup>2</sup>; Peter Jeschke<sup>2</sup>; Walter Wissdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>  
<sup>1</sup>University of Wuppertal, Wuppertal, GERMANY; <sup>2</sup>RWTH Aachen, Aachen, Germany

**Novel Aspect:** First experimentally validated three dimensional CFD model of a commercially available AP ion source, the Bruker MPIS

### Introduction

The numerical description of ion optical devices at atmospheric pressure (AP) requires valid and detailed computational fluid dynamic (CFD) models of the flow conditions in the device. The basic validity and applicability of the CFD model along with the specific model assumptions need to be validated experimentally. To the best of our knowledge, the whole CFD modeling process (model definition, spatial discretization, model optimization, and model validation) has not been demonstrated yet for a complex AP ion source geometry. However this approach represents a prerequisite for more advanced simulations of the dynamics in an AP ion source. The Bruker Multipurpose Ion Source (MPIS) was used as a test case.

### Methods

The numerical calculations were performed by conducting steady state simulations with a commercial CFD solver. A two-equation turbulence model has been used for closure of the RANS equations. An extra transport equation enabled the spatial resolution of the analyte gas within the ion source and therefore the mixing process of the nebulizer gas flow containing the analyte and the dry-gas was simulated as well. For validation of the numerical model, experimental data acquisition has been performed. Particle Image Velocimetry (PIV) experiments were chosen due to the detailed resolution of the flow field at minimized disturbance of the flow field. The pre-test prediction of the CFD results showed that PIV measurements are an adequate method to resolve the main flow features.

### Preliminary Data

Very recently we have demonstrated the general approach of modeling ion trajectories at viscous flow conditions using a setup with a rather simple geometry, which is characterized by essentially laminar flow conditions (ASMS conference abstract submitted). It was shown that the particle tracing software SIMION including the SDS extension and home-made custom software along with an accurate CFD model reproduces experimental results very well. The present approach goes far beyond the challenges of the laminar flow test-setup. Here we are using a Bruker MPIS as the experimental platform. Simple ion current measurements are not adequate for a validation of the corresponding model results. Instead, PIV measurements were used; the results yield much more directly related figures of merit with regard to the flow dynamics inside the MPIS. Initial numerical and experimental results clearly show the general validity of the modeling process. All important experimentally determined features of the flow dynamics in the ion source are reproduced by the numerical model after fixation of some distinct critical model boundary conditions. In addition, the relative neutral analyte density is calculated. It becomes clear that the relevant overall flow conditions in the ion source are critically determined by the fluid dynamical properties of the dry gas flow. This is surprising, since generally the nebulizing gas flow is dominating with respect to contributions to the total source gas flow. We present a detailed CFD model of a commercial AP ion source, i.e., the Bruker MPIS along with an experimental validation of the modeling results. A detailed discussion on the special features of the fluid flow in the ion source, the details of the experimental verification of the CFD model, and some general conclusions for AP ion source design is given.

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Poster: TP04 - New Developments in Ionization II, poster number: 070, Tuesday, Poster Hall

### **Comparison and Validation of Atmospheric Pressure Ion Migration Models - Finite Elements Method vs. Discrete Particle Tracing**

Klaus J. Brockmann; Walter Wissdorf; David Mueller; Sonja Klee; Valerie Derpmann; Sebastian Klopotoski; Thorsten Benter  
*University of Wuppertal, Wuppertal, GERMANY*

**Novel Aspect:** First direct comparison of two modeling approaches for ion motion at AP and experimental validation of the numerical results

### Introduction

The simulation of ion trajectories at complex fluid dynamical conditions remains a tough challenge. Nevertheless, significant progress in this area is of paramount importance for the development and optimization of atmospheric pressure ion sources and ion transfer systems. The prevailing high collision rates require careful modeling of the viscous interactions between ions and bulk gas. There are two established numerical methods commercially available, the finite element method (FEM) and discrete particle tracings with statistical diffusion simulation (SDS). To the best of our knowledge, a direct comparison of the performance of both methods has not been published. We present a comparison of FEM and SDS calculations for a simple benchmark problem along with an experimental validation of the numerical results.

### Methods

The FEM program package COMSOL Multiphysics was used for fluid dynamical and ion migration simulations. The SIMION charged particle simulator with the SDS extension was used for discrete ion migration tracings. All simulations were performed on a Dell Precision T7500 workstation. The interface layer for the data exchange between the software packages was developed in-house using multiple programming languages (Python, Lua, Matlab). The experimental verification was performed with a custom built experimental setup comprised of a dedicated vacuum chamber set-up, including a laminar flow tubular corona discharge inlet and Faraday plate ion current detector. The ion current was measured as function of flow dynamic and electrical parameters.

### Preliminary Data

The performance, required modeling effort, and the validity of the numerical modeling results regarding ion motion at viscous flow conditions are important figures of merit for further developments in this area. The approach presented here allows a direct comparison

of two fundamentally different modeling methods using a simple benchmark problem, which is validated with data obtained from a dedicated experimental set-up. In essence, a laminar bulk gas flow with charged species present, generated in a tubular corona discharge ion source located upstream, enters a considerably larger vacuum recipient equipped with a detection and a deflection plate. The gas flow is directed between the two plates and exits the chamber via an opposite port, which is actively pumped. The pumping speed is adjusted to maintain overall laminar flow conditions. Computational flow dynamical calculations clearly underline the laminar flow assumption. It is shown that the experimentally determined detection plate currents originating from ions generated upstream of the recipient are qualitatively reproduced by *both* numerical models. This holds true for the variation of fluid dynamical as well as the electrical forces. However, significant differences between the two modeling methods with regard to the required *modeling effort* and the *validity* of the numerical results are evident. The results demonstrate that we have established a reasonable test case for the direct comparison of a FEM based ion migration model in COMSOL and discrete ion tracings in SIMION/SDS. Currently, we are quantifying the details of the differences between the results from both numerical methods and the experimental measurements. The results of this quantitative comparison will be presented as well as an in-depth discussion.

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Poster: TP04 - New Developments in Ionization II, poster number: 075, Tuesday, Poster Hall

### Simulation of Ion movement in a 'long' gas dynamic interface

Andrew Entwistle<sup>1</sup>; Alina Andreyeva<sup>2</sup>; Sergey Bulovich<sup>3</sup>; Mikhail Lapushkin<sup>5</sup>; Alexander Bazhenov<sup>4</sup>; Roger Giles<sup>1</sup>; Nicolay Gall<sup>5</sup>  
<sup>1</sup>Shimadzu Research Laboratory, Manchester, UK; <sup>2</sup>Institute for Analytical Instrumentation, Saint-Petersburg, RU; <sup>3</sup>S.-Petersburg State Polytechnical University, Saint-Petersburg, RU; <sup>4</sup>VNIIOkeangeology Institute, Saint-Petersburg, RU; <sup>5</sup>Physico-Technical Institute, Saint-Petersburg, RU

**Novel Aspect:** Combined gas dynamic and ion optics

#### Introduction

Gas Dynamics plays important role in the ion transmission through any API interface region. Therefore detailed CFD simulation is necessary for realistic description of ion transport. Here simulation methods are illustrated by means of a basic gas dynamic interface consisting of first and second skimmers and DC lens. This system is characterised by the distance between the sampler outlet and the skimmer compared to the Mach barrel size. 3D CFD simulation are presented including detailed description of free expansion region and the downstream gas jet. Within this system ion movement is presented by considering the combined influence of electric fields and the gas flow. The results are compared to experimental data of the same system.

#### Methods

For production of the Gas dynamics field a 3D mode was calculated by Fluent 6.3, these results were converted to a uniform grid structure suitable for importing into ion optics simulation program, AXSIM. The electric field due to a DC focusing lens was calculated by SIMION 8.0. This lens was employed to focus ions towards the second skimmer. A hard sphere model was used to describe the collision between ions and gas molecules. The model system was chosen such that the distance between the sampler outlet and the skimmer was much greater than the Mach barrel size. For experimental comparison a the model interface was constructed and ions were analysed using TOF mass spectrometer.

#### Preliminary Data

The behaviour of the gas jet inside gas dynamic interface is affected very strongly by the length of the interface chamber: when it becomes much longer than the Mach barrel, the structure of the jet becomes stable with low turbulence. However, the behaviour of the gas jet depends strongly on the pressure in the interface, even if the above criterion of its 'length' is fulfilled. 3D CFD computations of gas jet structure have been made at pressures in the range 2 to 10 mbar. In general the jet structure was similar for all pressures: the Mach barrel ending with a shock wave; the region of transonic movement with the velocities of 300 - 450 m/s, and the region of subsonic movement where jet velocity is reduced. However, there are some significant differences in the jet structure due to the ambient gas pressure. The differences results mostly from the effectiveness of turbulent mixing of the jet with the ambient gas. At 10 mbar the jet velocity is reduced effectively to 50-70 m/s as it reaches the skimmer and is not strictly laminar (its turbulence viscosity ratio reaches a maximum of ~60). Whereas at 2 mbar the velocity of the jet remains high, 450 - 500 m/s up to the skimmer and no turbulence occurs. Regarding the DC focusing in the skimmer region preliminary simulation and experiments show that the dependence of ion transmission on the focusing voltage was found to be bell like with the optimum voltage increasing with ion mass and interface pressure.

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Oral: WOC pm - Fundamentals: Ion-Surface Interactions and Preparative MS, time: 3:50, Wednesday, Room 401

### The Study of Ion Transmission and Soft Landing of Macromolecules Using Multiple Quadrupoles Instrument Coupled with MALDI Ion Source

Ting-Chang Ko; Yao-Hsin Tseng; Wen-Ping Peng  
National Dong Hwa University, Shoufeng, Hualien, TAIWAN

**Novel Aspect:** Our homemade instrument can perform the experiment of ion transmission and soft landing of macromolecules using MALDI ion source.

#### Introduction

Most ion soft landing (SL) studies use electrospray ionization (ESI) or electrosonic spray ionization (ESSI) source as their ion sources. However, when macromolecules such as proteins or protein complexes are analyzed, the high charge numbers make the mass spectra very complicated and therefore cause the ion selection difficult. Moreover, ion transmission of most ion soft landing instruments is

limited to  $m/z$  value less than 4,000. In this study, we used matrix-assisted laser desorption/ionization (MALDI) as an ion source and used homemade multiple quadrupoles system to guide high mass MALDI ions, e.g. cytochrome c (CytC), into the quadrupoles system and the mass analyzer to achieve ion soft landing of C60 ions.

### Methods

The multiple quadrupoles instrument consists of four major components: a homemade square quadrupole (Q1), a 90-degree bent-square quadrupole (Q2) that can prevent the contamination of fast neutral molecules, a small square quadrupole (Q3) and a homemade rectilinear ion trap (RIT) as a mass analyzer with front and back end-cap lenses for ion trapping. The MALDI ion source was employed and the detector consisting of a conversion dynode and an electron multiplier was set on the lateral side of RIT. Soft landing surface was located behind the back end-cap lens. At last, the soft landed ions were analyzed using Bruker's MALDI time-of-flight (TOF) mass spectrometer (MS).

### Preliminary Data

Guided by three quadrupoles which was operated at rf only mode and was filled with cooling buffer gas, ions was then transferred to RIT. C60 was employed to calibrate the mass spectra of RIT mass analyzer. Two kinds of compounds were measured in ion transmission experiment. The first were polystyrene (PS) standards with the nominal molecular weight 800, 4000, and 13000. The second were peptides (angiotensin I, ubiquitin) and proteins (cytochrome c). Each mass spectrum of these ions could be obtained successfully by adjusting proper parameters. By lowering the resonance rf frequency, ion transmission of high  $m/z$  ions could be achieved, which could avoid the voltage limitations applied to quadrupoles (Q1, Q2, Q3). Currently, the  $m/z$  range of ion transmission can be extended to  $m/z \sim 12500$  (CytC) and the dimer signal at  $m/z \sim 25,000$  was also observed.

In addition, by raising the amplitude of rf voltage, we found the relative intensity of PS800 ions was decreased despite multiple quadrupoles were operated in rf only mode. The above experiment indicated that low mass cut-off of PS800 ions existed in the ion transmission experiment. Tuning the floating dc potential of quadrupoles could also reduce the ion signals in low  $m/z$  region. SIMION simulation of ion trajectories was done with geometry of the current setup. The simulation showed an ion transmission efficiency of high mass ions was about 98% even with  $m/z$  up to 10,000,000. Detailed analysis of the bent-square quadrupole was done by Poincare-Lighthill-Kuo (PLK) perturbation method and SIMION simulation and showed the ion transmission efficiency strongly depended on kinetic energy of guided ions.

Finally, the soft landed C60 ions were transferred to MALDI-TOF MS. The SL signal of C60 was obtained, which demonstrates our current setup can perform the soft landing experiment.

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Oral: WOE pm - Instrumentation: New Developments in Instrumentation, time: 3:30, Wednesday, Korbel Ballroom 3-4

### Incorporation of Surface Induced Dissociation into an Ion Mobility – QTOF Mass Spectrometer for Post-Ion Mobility Activation

Mowei Zhou<sup>1</sup>; Chengsi Huang<sup>1</sup>; Kevin Giles<sup>2</sup>; Anne Blackwell<sup>1</sup>; Vicki Wysocki<sup>1</sup>  
<sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Waters Corporation, Manchester, United Kingdom

**Novel Aspect:** This work presents the first implementation of SID into a commercial ion mobility QTOF mass spectrometer.

### Introduction

Surface induced dissociation (SID) has been observed to have different fragmentation behavior from collision induced dissociation (CID) that provides complementary information for structural analysis, especially for non-covalent protein complexes. Ion mobility (IM) has recently gained popularity on separation of biological molecules by their collisional cross sections in gas phase. Introducing IM separation before or after ion activation will definitely expand the application of SID in solving more complicated structural problems. A home-made SID device has been installed into a modified commercial Q-TOF instrument with IM capability (Waters Synapt G2<sup>®</sup>). The inserted SID device, which is after the IM cell in the current setup, enables SID on mobility separated analyte ions in addition to the post-IM CID in the original instrument.

### Methods

Simulation of the SID device was done using SIMION<sup>®</sup> to determine the effect of lens geometries on ion transmission. The device was fabricated and modified at the University of Arizona. The original transfer T-wave ion guide in the instrument was shortened to accommodate the SID device. The voltages on the lenses of the SID device are controlled by an external power supply to achieve either a fly-through transmission, or collision with the surface and subsequent collection of fragment ions. Several common peptides, cesium iodide clusters and protein complexes with known CID/SID behaviors from previous experience in the PI's laboratory were used to test the performance of the modified instrument.

### Preliminary Data

The SID design was adapted from the previous generation of SID in a QTOF2 instrument with some changes to geometry and dimension. SIMION<sup>®</sup> simulations showed that ion transmission can be maintained in the new design. The SID device was then fabricated and installed into the modified Waters Synapt G2<sup>®</sup>. C-reactive protein (CRP), serum amyloid P (SAP) and transthyretin (TTR) were used to check the SID capabilities of the modified instrument without IM separation. CID of CRP pentamer, SAP pentamer and TTR tetramer showed typical highly charged monomer and complementary (n-1)-mer fragments. In contrast, SID predominantly results in monomer fragments with evenly distributed charge. These observations are consistent with previous studies of SID from the PI's laboratory, confirming the successful installation of SID in the modified Synapt.

IM separation of a reverse peptide mixture (SDGRG and GRGDS) and a mixture of desR1/desR9 bradykinin (PPGFSPFR and RPPGFSPF) has been achieved with subsequent CID/SID. Each species in the mixtures was identified by its b/y ion series in post-IM CID and SID spectra. Cesium iodide clusters (CsI)<sub>20n</sub>Cs<sub>n</sub><sup>nt</sup> (n=1-5) with overlapping  $m/z$  were separated by IM and then activated by

CID or SID. Loss of multiple neutral Csl units was the major pathway observed by CID, while SID showed a significant amount of charge separation generating smaller cluster ions. The result illustrates the possibility of activation by CID/SID on mobility separated ions for clusters and more complicated samples.

TTR tetramers were activated by in-source collision at elevated cone voltages. Preliminary data suggests that tetramer species with elongated drift times result in a less symmetric fragmentation pattern by SID. However, there was no significant differences in CID fragmentation pattern for the pre-activated tetramers.

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Oral: WOE pm - Instrumentation: New Developments in Instrumentation, time: 3:50, Wednesday, Korbel Ballroom 3-4

### **Design and Simulation of a Miniaturized Zaifman Trap for Electrostatic Storage of Ions with < 1 keV of Energy**

Ryan T. Hilger; Robert E. Santini; Scott A. Mcluckey  
*Purdue University, West Lafayette, IN*

**Novel Aspect:** A miniaturized Zaifman trap for high resolution mass spectrometry of ions with less than 1 keV of energy.

#### **Introduction**

Zaifman traps are electrostatic devices previously shown to be effective at storing energetic ions. Zaifman traps exhibit a remarkable phenomenon, termed self-bunching, in which the spacial distribution of ions within an ion packet remains constant as a function of storage time. Self-bunching allows a Zaifman trap to be used as a high resolution Fourier transform mass spectrometer. Previously constructed Zaifman traps have lengths approaching one-half meter and store ions with energies of several keV. We have designed a trap that is less than six inches long and is optimized for storage of ions with a few hundred eV of energy. We demonstrate the performance of our device using SIMION simulations and establish that our trap will be capable of self-bunching.

#### **Methods**

Ion trajectory simulations were performed using SIMION 8.0.

#### **Preliminary Data**

Our trap is designed such that it can be constructed primarily from off-the-shelf components. The trap consists of little more than metal plates spaced by ceramic beads. The potentials applied to the plates span a range of less than 1 kV when ions with energies of 420 eV are stored. An ion with  $m/z = 100$  Da has an oscillation period of about 10  $\mu$ s.

Self-bunching occurs because of interactions between the ions in a bunch when they slow down near the turning point at each end of the trap. In order for self-bunching to occur, it has been shown that the spread in the ions' arrival times at the turning point,  $\Delta t$ , must be minimized. The time spread may be calculated using the following equation:

$$\Delta t = (\Delta t_a^2 + \Delta t_v^2)^{1/2}$$

Where  $\Delta t_a$  is the time spread due to the variation in the lengths of the paths taken by ions of identical energy, and  $\Delta t_v$  is the time spread due to the energy distribution. Past work has shown that  $\Delta t$  values in the sub-nanosecond range are required for self-bunching. Practically,  $\Delta t_v$  can be made vanishingly small by adjusting the potentials such that ions with higher energies take longer paths, similar to what occurs in a reflectron. In addition,  $\Delta t_a$  can be minimized by adjusting the potentials so that only ions travelling very near the axis are trapped. Ion trajectory simulations show that, by properly adjusting the potentials, it is possible to flip the sign of  $\Delta t_v$ , demonstrating that its magnitude can be made extremely small. We also show that  $\Delta t_a$  can be reduced below 1 ns when the potentials are adjusted such that only ions within 0.3 mm of the axis are trapped.

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Poster: ThP02 - Instrumentation: General, poster number: 020, Thursday, Poster Hall

### **A new numerical code for calculation of electric field and simulation of ion motion in FT-ICR with arbitrary electrode geometry**

Alexander Misharin<sup>1</sup>; Alexander Popov<sup>2</sup>  
<sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>MSU, Moscow, Russia

**Novel Aspect:** Novel numerical code for calculations of electric fields from arbitrary shaped electrodes and simulation results for optimized O-trap geometry

#### **Introduction**

Computer experiment in FT-ICR mass spectrometry plays an increasingly important role. It requires utilization of the tools adequate to simulate very complex nature of real FT-ICR experiment. Over the past several years parallel numerical code PIC3D for supercomputer simulation of the ion motion dynamics in FT-ICR cells was created[1]. Finite difference methods used to obtain solution of the Laplace equation in PIC3D and other software (SIMION, Mitchell's implementation of the 3D particle-in-cell code[2]) generally give correct results for closed electrode surfaces only. Our new "T-field" numerical code alleviates this limitation by using method of solution for potential based on boundary equations of potential theory. "T-field" code can calculate electric field for any configuration of unclosed electrodes with arbitrary geometry.

## Methods

Method of electric field calculation implemented in the "T-field" code is based on solution of integral boundary equations of potential theory. This method permits one to calculate electric field from electrodes of arbitrary geometry. Also, influence of gaps between the electrodes can be taken into account. Electric potentials can be calculated on any irregular grid mesh inside the FT-ICR cell which permits one to have desired field precision in different regions of the cell.

## Preliminary Data

New version of the PIC3D code which uses electric field configurations calculated by "T-field" was created and implemented on IBM Blue Gene/P supercomputer (computation speed 28 TFLOPS). New "T-field"/PIC3D software was used for optimization of the excitation compartment of O-trap FT-ICR cell [3]. A novel configuration of electrodes in the excitation compartment which makes excitation field profile close to the ideal one was found. Simulation of the ion cloud motion in the excitation compartment for different excitation protocols (single frequency, SWIFT) was performed. Along with the results for optimization of the excitation compartment, bench mark calculations and simulations of the ion motion in the detection compartment of the O-trap cell will be presented. [1] E.N. Nikolaev, A.M. Popov, R.M.A. Heeren, et. al.; *Rapid Commun. Mass Spectrom.* 2007, 21, 3527. [2] D.W. Mitchell; *J. Am. Soc. Mass Spectrom.*, 1999, 10, 136. [3] A.S. Misharin, R.A. Zubarev, V.M. Doroshenko; *Rapid Commun. Mass Spectrom.* 2010, 24, 1931.

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Poster: ThP02 - Instrumentation: General, poster number: 022, Thursday, Poster Hall

### Development of a Periodic-focusing DC Ion Funnel and Accumulation Device for an Electrospray Ionization Source

Kyle L. Fort; Joshua A. Silveira; David H. Russell  
*Texas A&M University, College Station, TX*

**Novel Aspect:** A novel electrostatic ESI ion funnel and accumulation device base upon periodic focusing is discussed.

#### Introduction

Sensitivity of Electrospray Ionization (ESI) in mass spectrometry-based studies is limited by the conductance of ions from the high-pressure source region into the vacuum of the spectrometer. In order to increase the sensitivity, ion funnels are typically used to focus and accumulate ions at the entrance of the spectrometer. Ion funnels are typically constructed using a series of decreasing inner diameter electrodes and radio frequency (RF) potentials to radially focus the ion trajectories. Recently we have shown that periodic-focusing DC (PDC) potentials can be used to radially focus ion trajectories in an ion mobility drift cell. Work shown here follows the development of a PDC -based ion funnel (PDC IF) with an ion accumulation device in combination with ESI.

#### Methods

Simulations are performed using SIMION 8.0 from Scientific Instrument Services. Ion trajectories are modeled using the collision\_hs1.lua program within the SIMION software. Several different model ions are used including varying charge states of Cytochrome C and C60. Previously reported collision cross section (CCS) values are used in the simulations. Pressure conditions of 0.75 torr to 1.25 torr are investigated for ion transmission to simulate actual operation conditions within an ESI source. Ion transmission is calculated for the model compounds at varying operation parameters. The neutral collision gas used in these simulations was helium.

#### Preliminary Data

The PDC IF and accumulation device consists of three sections. The first section utilizes a series of decreasing inner diameter electrodes in order to radially focus the ions from the heated capillary. The second region is a series of expanding inner diameter electrodes allowing for ion accumulation; followed by the third region, which refocuses ions with decreasing inner diameters. Preliminary simulation studies are carried out by introducing ions into the entrance of the funnel with 2000 kV extraction voltage. The ion transmission through the device is upwards of 90% with 1 torr of helium. Simulations are conducted to investigate the feasibility of introducing ions orthogonally to the ion funnel and accumulation device. Orthogonal ion electrospray conditions are preferred to minimize the introduction of air into the PDC IF since the optimal operation of PDC IF is demonstrated with low- molecular-weight gases such as He. Several orthogonal introduction techniques are explored using C60. Once a final extraction technique is determined, the transmission of model ions is calculated. At 0.75 torr the average C60+ transmission through the device is 78%; however, when multiple charge states are explored, the ion transmission increases. An ion with a mass of 720, a charge state of +6, and a CCS of 124 Å<sup>2</sup> has an average transmission of 91% when introduced orthogonally to the funnel; additionally, higher charge states of a 720 mass ion with the same CCS have greater than 90% transmission. Overall, the series of +1 to +11 charge states were modeled and the average transmission is 89%. When the pressure is increased to 1 torr, the average transmission for the +1 to +11 series is 95%; additionally, for 1.25 torr simulations, the series has a 91% transmission. Various charge states of Cytochrome C are also modeled with >90% ion transmission.

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Poster: ThP02 - Instrumentation: General, poster number: 023, Thursday, Poster Hall

### Dynamics Simulation of Larger Molecules; Differential Mobility Analyzer with Newly Designed Mass Spectrometer Inlet

Yi She; Chenxi Zhu; Eiko Koizumi; Hideya Koizumi  
*Arkansas State University, State University, AR*

**Novel Aspect:** Study of aerosol dynamics and performance of new DMA through the computer simulation.

## Introduction

Current mass spectrometry technology allows analysis of particle size up to 700 kD safely. It is not easy to obtain high resolution mass spectra with existing mass spectrometer designs due to kinetic energies carried by larger-size molecules (1MD and beyond) at expansion. Our group recently developed a new design of high-pressure device, and we continue our effort on testing and improvements. The plan requires a theory (mathematics and physics) and highly accurate simulations for visualization and interpretation of the theoretical results. We discuss importance of aerodynamics within system with large body particles and present our new differential mobility analyzer which could potentially be coupled with mass spectrometers. The performance of the instrument is discussed based on computational results.

## Methods

As in our initial stage of large-molecule simulation, we added concepts of drag with slip corrections, relaxation time, molecular shape and its cross section and viscosity into statistical trajectory model currently commonly used. Molecules of larger sizes are released into a non-uniform velocity field calculated according to fluid dynamics (with Navier-Stokes equations) to obtain the time development of fluid packets rich in large molecules. Code for flow calculations and graphic interpretations are developed with COMSOL Multiphysics package. The flow field is imported into SIMON user program code specifically optimized for larger molecules. The performance of the DMA developed in a laboratory setting is tested under variable conditions.

## Preliminary Data

A built-in SIMION user program, "the Statistical Diffusion Model", was modified to give better approximations of motion of large (micron size) particles. Standard temperature and pressure were used for all models. Several case studies of particle trajectories were calculated that show development of stationary particles in response to several variables including moving uniform air, pipe flow, applied voltage, and impaction, were analyzed and shown to be consistent among all cases studied. Flow field calculated by COMSOL Multiphysics package with relatively simple grid system showed fully developed laminar flow acceptable as our simulation condition despite some complication arise from electrode geometry. Therefore, the result was imported into SIMION program without further refinements and improvements. At point source upstream, packets of poly-dispersed particles with randomly fluctuating concentrations with known average concentration were released. Only singly charged particles were generated to mimic the approximate charge distribution produced by typical discharger. The voltage scan functions are programmed through user interface to control the size by electric mobility. Recorded spectra of ion mobility showed some improvements in resolution. Transfer functions obtained by computer simulations showed improved efficiency in new DMA design as its analytic formulation predicted. Reduction in resolution and transfer efficiency by diffusion spread was observed as it is typically the case in any ion mobility device. Over wide range of experimental parameters and particle masses were tested for newer design and theoretical spectra shows promising technology for future mass spectrometry inlet.

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Poster: ThP02 - Instrumentation: General, poster number: 024, Thursday, Poster Hall

## High Dynamic Range Ion Detection Using Channel Electron Multipliers

Paul Mitchell; Stephen Ritzau; Lenny Erickson  
*Photonis USA, Inc., Sturbridge, MA*

**Novel Aspect:** A new compact, circular symmetry dynode design allows small size and significant improvement in dynamic range, without compromise to longevity.

## Introduction

Channel electron multipliers (CEM) have widespread use for ion detection in Mass Spectrometers due to their high sensitivity and small size. However, the voltage gradient inside the channel is not stable at high output current, limiting the dynamic range of the CEM. Such stabilization is a common feature of discrete-dynode electron multipliers. Channel Electron Multipliers are uniquely suited to the addition of several stages of discrete-dynode sections to permit higher current output levels. By proper design of the dynode section, the overall size of the detector can remain physically very small, while extending the dynamic range of the instrument.

## Methods

This work is based on a six pore spiral configuration CEM where the electrons are confined to a small, radially symmetric exit region. Simion electron optics was used to set the dynode shapes to allow optimal coupling as well as the ideal electron flow from stage to stage. Once the dynodes are configured, the materials to be deposited onto the active surface for secondary emission were developed to achieve the added gain and current handling. In addition, the gain setup and bias method can be decided with a view towards simplifying the application of the detector in the field.

## Preliminary Data

Earlier work, based on a five stage multiplier, has proven the feasibility of this approach, but at a prohibitively high cost. As an alternate, the discrete-dynode assembly was reduced in dynode number and its collection efficiency improved.

The gain achieved by discrete dynodes depends upon materials used to create secondary emission and the process by which the materials are applied. So far, the results for secondary emission of a single stage have been measured at 2.2X at 75 volts and up to 3.6X at 150 volts. For a three stage multiplier combination, we expect to achieve gains in the range of 10X to 42X overall.

The bias arrangement for the discrete dynodes follows the usual channel electron multiplier plan for grounded anode and negative high voltage. The extra voltages required by the discrete dynodes are formed by a resistive divider with small capacitors to stabilize the

voltages during high current pulsed outputs. Techniques to bias the combination have been found that may allow gain settings to be more consistent.

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Poster: ThP02 - Instrumentation: General, poster number: 026, Thursday, Poster Hall

### Computer Simulation of Ion Trajectories in Atmospheric Pressure Electrospray Ionization (AP-ESI)

Kenichiro Saito<sup>1</sup>; Yury Dessiaterik<sup>2</sup>; Eiko Koizumi<sup>1</sup>; Hideya Koizumi<sup>1</sup>  
<sup>1</sup>Arkansas State University, State University, AR; <sup>2</sup>Colorado State University, Fort Collins, CO

**Novel Aspect:** The computer simulation provides insight to complicated electrospray phenomenon during drying stage.

#### Introduction

Electrospray ionization (ESI) generates highly charged droplets through process of producing the gas phase ion from charged droplets at high pressure condition. It has been frequently used in mass spectrometry as preferred ion source and made a large contribution to both industry and academics. Despite its importance and usefulness, its mechanism has not been completely understood due to a variety of phenomena such as evaporation, fission and aerodynamic drag affects that complicate simulations. We studied the process by a computer simulation for which may provide insight into the process mechanism and contribution to potential development of new designs and future mass spectrometry technology.

#### Methods

Initially, charged droplets are placed near the tip of a Taylor cone under typical electric field setting in electrospray. The evolution of droplets is tracked and recorded. The rate of evaporation and fission were controlled by temperature, charge, and surface tension of droplets using applied Maxwell's equation and Rayleigh limit with probabilistic variations due to irregular shapes. Each splitting of charged droplets is modeled as "multiple daughter droplets fission process". The statistical variations are also implemented here. The daughter droplets are estimated to have 1/10th of the pre-splitting radius. The droplets undergo fission process several times during the drying stage.

#### Preliminary Data

Aerodynamic parameters were implemented to obtain trajectories at high pressure condition by SIMION software package. The initial charge carried by droplets were assigned to be approximately 80% (random fluctuation is given by the program) of the instability limit. Because of the presence of sheath gas flow, trajectories of droplets were simulated under the presence of both diffusional and pressure force by the flow of gas. The weak nitrogen flow with low Reynolds number was used to avoid known complications such as convective heat transfer at this stage of the modeling. The narrow beam of droplet particles broadened as away from the tip of syringe needle as expected to form a plume. The Coulomb repulsions between droplets and pressure gradients pushed the droplet away from the center of the plume. Smaller droplets were found typically on the outside the plume flow due to their small inertia and we saw that in our simulations. The fission process was modeled by several different methods, and the beam (plume) shapes varied by methods. Variations in initial distributions of the droplets also affected the plume flow development. Several different solutions have been applied for ESI where water produced slightly narrower plume than ethanol solution. Finally, the temperature of liquid is controlled by the initial temperature at initial state. The model predict faster diffusive split in this simple electrospray ionization model regardless of the surrounding conditions.

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Poster: ThP03 - Instrumentation: New Concepts, poster number: 042, Thursday, Poster Hall

### A Periodic-focusing DC Ion Funnel Interface for a Variable-temperature Ion Mobility Spectrometer

Joshua A. Silveira; Chaminda M. Gamage; David H. Russell  
Texas A&M University, College Station, TX

**Novel Aspect:** Simulation-based development and experimental results for characterization of an electrostatic periodic-focusing DC ion funnel (PDC IF) are reported.

#### Introduction

Radial diffusion adversely affects IMS ion transmission and results in reduction of the overall instrument sensitivity. Several strategies utilizing inhomogeneous RF fields have been employed to improve ion transmission; however, our laboratory has shown that an analogous effect may be achieved utilizing only DC potentials applied to periodic-focusing electrodes. We previously reported the major transport properties of a periodic-focusing DC ion guide (PDC IG) which include *axial drift* giving rise to IMS separation, as well as *radial ripple* and *central drift* motion owing to an effective RF and an ensuing effective potential acting upon the ions, respectively [1]. Here, we demonstrate the versatility of a periodic-focusing DC ion funnel (PDC IF) operating inside of a variable-temperature ion mobility spectrometer.

#### Methods

The geometry of the PDC IF was optimized by simulation of ion trajectories using SIMION.  $C_{60}^+$  ion trajectories were modeled using the *collision\_hs1.lua* program provided with SIMION to study hard sphere collisions with helium at temperatures between 298-78 K. The PDC IF was incorporated into a 30 cm variable-temperature IMS drift tube and initially tested at pressures between ~0.5-2 Torr.

Experimentally, fullerene ions are generated via laser desorption ionization (LDI) using a pulsed Nd:YAG ( $\lambda = 353 \text{ nm}$ ,  $f = 200 \text{ Hz}$ ) and focused into the drift tube through a series of electrostatic lenses. Ions traverse the drift tube under *low-* or *intermediate-field* conditions and are measured using an in-line detector.

### Preliminary Data

In the variable-temperature drift tube, the first 22 ring electrodes generate a uniform electric field while the last three electrodes provide periodic-focusing fields to facilitate ion transport through the exit aperture to the detector. Electrically, the PDC IF may be biased independently from the uniform field segment or connected to the drift tube through an external resistor. Simulation results have demonstrated that independent tuning of the PDC IF can greatly enhance ion transport through the drift tube exit aperture while alternatively, an identical net electric field across the drift tube and PDC IF segments becomes important when accurate collision cross-section values are desired.

Moreover, the simulation results indicate that the PDC IF can be easily adapted toward high transmission or high resolution applications, depending on the electrode geometry. In this case, maintaining high resolution with a modest gain in transmission is preferable. The simulation results show that at cryogenic temperature, a small PDC IF constructed from only 3 electrodes can transmit ~58% of the ions through a 30 cm drift cell while maintaining IMS resolution ~68. These findings indicate a substantial improvement in ion transmission through the IMS interface which typically yields ~10% transmission at cryogenic temperature.

Initial experimental studies have centered upon investigation of PDC IF operating conditions at ambient temperature. Separation of  $\text{C}_{60}^+$  and  $\text{C}_{70}^+$  is demonstrated under *low-field* IMS conditions. Future experiments will focus on low temperature IMS measurements, analysis of peptide and protein ions, as well as determination of ion-neutral collision cross section using the IMS-PDC IF instrument.

[1] Gamage, C. M.; Silveira, J. A.; Blase, R. C.; Russell, D. H. Gas-phase Ion Dynamics in a Periodic-focusing DC Ion Guide (Part II): Discrete Transport Modes. *Int. J. Mass Spectrom.* In Press.

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Poster: ThP03 - Instrumentation: New Concepts, poster number: 044, Thursday, Poster Hall

### Considerations for the Design of an 8-Channel Spatially Multiplexed Ion Mobility-Mass Spectrometer

Jody May; Sevugarajan Sundarapandian; Kyle Osborne; John A. Mclean  
Vanderbilt University, Nashville, TN

**Novel Aspect:** Instrument details for an ion mobility-mass spectrometer constructed with eight parallel channels for high-throughput analysis and experimental versatility.

### Introduction

Spatial multiplexing strategies are common in sample preparation (96-well plates, microarrays and 2D gels) prior to MS analysis. Multiplexed prefractionation and sample delivery (multiple LC columns, arrayed electrosprays) have also been described. Parallel sampling improves statistical relevance and overall sample throughput, allowing more experiments with higher confidence results. As the front-end sampling is streamlined, the analyzer becomes the rate-limiting step. Operating several spectrometers in parallel is one solution, but this is oftentimes prohibitive in terms of monetary costs, maintenance investment and availability of laboratory space. One novel but challenging solution is to develop a multi-channel spectrometer in the footprint of a single-channel instrument. Here we describe the considerations for an 8-channel ion mobility-mass spectrometer currently being constructed for high-throughput analyses.

### Methods

The 8-channel ion mobility-mass spectrometry (IM-MS) instrument is comprised of (i) an electrospray ionization (ESI) source array of 8 emitters and 8 heated capillary tubes, (ii) an 8-channel ion funnel array utilizing a "keyhole" design for simultaneous ion focusing, accumulation and release into (iii) an IM spectrometer array comprised of 8 spatially discrete channels, (iv) a converging array of 8 ion funnels to recollect ions, (v) 8-channel vacuum ion optics to transition beams into vacuum and shape/steer ions for injection into (vi) an orthogonal time-of-flight MS equipped with (vii) a spatially-resolved discrete anode detector array. The ion source, IM spectrometer and funnels are being designed and constructed in house. The time-of-flight MS is being modified from commercial instrumentation (QSTAR, AB/Sciex).

### Preliminary Data

The instrument is designed in modules such that each component can be independently tested. Instrument components are designed in silico using SIMION 8 and CAD software. Theoretical instrument performance is calculated from fundamental equations. Funnel and the IM spectrometer are constructed from stacked electrode strips spaced with insulating sheet. Each electrode strip is comprised of 8 holes such that the entire 8-channel assembly shares a common vacuum system and electronics. The source ion funnel geometry is replicated from a previously optimized design. The converging ion funnel compresses the 8-channels from the IM into a small area amendable to the ion optics of the commercial TOFMS. Simultaneously, the converging array focuses ions radially. The performance of this array is evaluated in terms of transmission and temporal spread of post-IM ion packets, and a converging funnel design is presented which matches near 100% ion transmission with a modest loss in IM resolving power. The IM spectrometer dimensions (25mm ID, 30cm length) are balanced between high transmission (nondestructive radial ion diffusion) and good resolving power (ca. 30-50). Considerations for minimizing channel cross-talk through proper instrument design and operation is also discussed. The orthogonal TOFMS is critically evaluated with ion simulations in order to maintain discrete beam trajectories. Channel mixing is shown to be dependent on field uniformity and acceleration fields utilized. Higher voltages minimize ion dispersion at a modest cost of

instrument performance. Modifications to the commercial TOFMS are presented which allow higher voltage operation. Finally, the design of an 8-channel ion optics assembly is presented which allows independent focusing, steering and shaping of discrete ion channels prior to introduction into the TOFMS. The setup for 8-channel data acquisition has been designed and will be briefly mentioned alongside some prospects for the novel impact of this instrument on fundamental and applied research.

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Poster: ThP03 - Instrumentation: New Concepts, poster number: 045, Thursday, Poster Hall

### **Development of a Helical Dipole-based Atmospheric Interface Setup for Enhanced Ion Transfer Efficiency**

Tamas Majoros<sup>1</sup>; Daniel Szalay<sup>2</sup>; Gyorgy Hars<sup>3</sup>; Zoltan Takats<sup>4</sup>

<sup>1</sup>*Semmelweis University, Budapest, HUNGARY*; <sup>2</sup>*Medimass Ltd., Budapest, Hungary*; <sup>3</sup>*Budapest University of Technology and Economics, Budapest, Hungary*; <sup>4</sup>*Justus-Liebig-University, Giessen, GERMANY*

**Novel Aspect:** A novel type of atmospheric interface was developed, which provides significant enhancement of ion transfer efficiency for various ionization methods.

#### **Introduction**

Atmospheric interfaces are indispensable parts of any instrument employing atmospheric pressure ionization methods, including electrospray or atmospheric pressure chemical ionization. The basic function of an atmospheric interface is to transfer ions from atmospheric regime of instrument to the analyzer region. Ideally, an atmospheric interface is expected to maximize the number of transferred ions while minimizing the number of neutrals transferred to vacuum system. Currently used interface setups, however achieve 0.01 – 5% ion transfer efficiency with 0.01-0.05 SCFM air load on the system. Poor transfer efficiency is generally attributed to ion neutralization and mobility effects. A novel interface setup employing helical dipole ion conduit is proposed to minimize or completely eliminate these effects.

#### **Methods**

A helical dipole ion guide was constructed by wrapping a double helix of electrodes around plastic (PVC) holder. Plastic was removed by dissolving it in THF. The helix was accommodated into the atmospheric interface of a ThermoFinnigan LCQ mass spectrometer. Resulting experimental setup contains an inlet capillary, the helical ion guide (a pair of helix-shaped electrodes in a coaxial arrangement with a symmetrical RF voltage applied). The capillary ends inside of the helical ion guide injecting ions directly into the retaining field. Without making any change in the cross section of the ion guide, the ions can pass through the second conductance limit. Ions are then injected directly into the following ion optic element, in this case a flatapole.

#### **Preliminary Data**

Both a linear and a curved version of the helical ion guide was built and tested. Comparison was made between the commercially available setup and our setup containing the helical ion guide regarding ion transfer efficiency, gas conductance and mass discriminations. The results show significant (1-2 orders of magnitude) increase in ion transmission depending on the actual ionization and ion source setup used. The ion guide was found to show mass discrimination under certain conditions. Mass discrimination effects depend on the driving frequency and amplitude of RF. The mass selective capabilities were more definite compared to the original (commercially available) setup, thus the ion guide could also be applied as a more effective mass pre-filter. The effect of geometry imperfections was examined, and the setup was found to be robust and stable even with some serious artificial imperfections in the thread of helix. The signal to-noise-ratio (SNR) also increased, especially in the case of the curved version. One of the particularly interesting areas of application of the device is its combination with ambient ionization methods, such as desorption electrospray ionization (DESI) or rapid evaporative ionization (REIMS). Helical ion guide device was tested with DESI and ~ 70 – 90 x signal intensity enhancement was obtained, which generally solves the problems associated with the poor ion yield of the ionization method. The helical ion guide provides a geometrically more open setup for ion transfer resulting in more efficient effusion of neutrals out of the device. In case of curved helix, transfer efficiency of the device for neutrals is practically zero while ion transfer efficiency is > 97% as it was successfully modeled in SIMION. This feature allows larger gas conductance on the first conductance limit, which results in further enhancement of the overall sensitivity of the instrument.

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Poster: ThP03 - Instrumentation: New Concepts, poster number: 054, Thursday, Poster Hall

### **FTIR Experiments on Mass Selected Cations by Counter-Ion Introduction Into an Inert Argon Matrix**

Nathan Roehr; Jan Szczepanski; Nicolas Polfer  
*University of Florida, Gainesville, FL*

**Novel Aspect:** Controlled introduction of counter ions for matrix isolation experiments.

#### **Introduction**

Obtaining infrared absorption spectra of cations is a challenging endeavor due to the low densities that can be achieved in the gas phase. In matrix isolation, ions of interest are accumulated in a cold inert matrix of a rare gas (e.g. argon) until sufficient concentrations are attained for direct spectroscopic characterization.[1] Nonetheless, in order to ensure neutralization of the matrix, experimentalists

often rely on non-ideal, energetic processes, such as electron emission from metal surfaces upon cation bombardment.[2] A better method for matrix neutralization would involve co-depositing a molecular counter-ion. Here, we present a two-ion source instrument to deposit cations and anions simultaneously into a cold inert matrix.

## Methods

A custom-made high-emission current electron ionization (EI) source (Ardara Technologies), custom quadrupole deflector bender (built in-house), and quadrupole mass filter (Balzer) generate low nanoAmp currents of mass-selected cations. A chemical ionization (CI) source (Finnigan 4500) generates low nanoAmp currents of anions. The two ion beams are merged into an octopole ion guide via a second quadrupole deflector bender (Ardara Technologies). The two beams are deposited onto a copper window, cooled to 12K by a helium cryostat. At the same time, argon is leaked into the vacuum chamber to form a matrix of solid argon on the cryostat window. A MIDAC 2000 FTIR spectrometer is used to measure IR absorption spectra of the ions.

## Preliminary Data

The target molecules of interest are naphthalene ( $C_{10}H_8$ ,  $m/z$  128) and adamantane cation ( $C_{10}H_{16}$ ,  $m/z$  136). 3-4 nA of mass-selected precursor ions could be generated using the EI source and transported to the second deflector. Using the CI source 1-2 nA of  $SF_6^-$  anions ( $m/z$  146) could be produced. Initial testing experiments aim at measuring FTIR spectra of known ions, Naphthalene cation is known to exhibit strong bands at 1215 and 1216  $cm^{-1}$  while  $SF_6^-$  displays bands at 594  $cm^{-1}$ . [3,4]

Preliminary experiments have shown that either ion beam could be directed efficiently onto the cryogen window. Simultaneous deposition of both ion beams resulted in near zero current, as both beams may neutralize each other at the surface, this needs to be verified by FTIR absorption measurements. In this sense, the presence of two IR-active ions in combination with linear absorption spectroscopy, are useful to confirm ion densities.

We have also simulated the two ion beams traveling through the quadrupole deflector using SIMION. In these simulations, the cations were biased at +10 VDC, while the anions were biased at -110 VDC. By employing an asymmetric ion bias, it is possible to explore different trade-offs in the experiment. Low bias voltages complicate efficient ion transmission of opposite polarity through a quadrupole deflector. However, a large ion bias potentially results in dissociation upon ion deposition in the matrix. For strongly bound cations, such as naphthalene, this may not present a problem.[1] For more fragile cations, such as the adamantane radical cation, this may constrain experimental conditions.

1. Maier, *et al.* J. Chem. Phys. **90**, 600(1989).
2. Godbout, *et al.* J. Phys. Chem. **100** 2892-2899(1996).
3. Szczepanski, *et al.* J. Phys. Chem. **96**, 7876-7881(1992).
4. Barefield, *et al.* J. Phys. Chem. **81**, 634-636(1977).

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Poster: ThP03 - Instrumentation: New Concepts, poster number: 061, Thursday, Poster Hall

## New Ion Trap Designs Obtained from Mapping Stability Diagrams and Determining Secular Frequency of Ion Oscillation Using Simion®

Joe Oliphant; Edgar Lee; Steve Lammert  
*Torion Technologies, Inc, American Fork, UT*

**Novel Aspect:** A novel method to gauge the degree of field nonlinearities on ion behavior in novel ion trap designs is discussed.

### Introduction

The trapping potentials for commonly encountered ion traps (e.g., the linear ion trap and the Paul trap), can be characterized using multipole expansions of the electric field. For a given device, the terms in the multipole expansion are useful for predicting ion behavior and describing differences in different geometries. Unfortunately, it has proven difficult to obtain multipole expansions for traps of other geometries, for example the toroidal ion trap. A mathematically less challenging and more robust method of analyzing ion traps of arbitrary geometry and optimizing their electric fields is needed.

### Methods

A novel approach using Simion has been developed that allows mapping the stability diagram of ion traps of arbitrary geometry. The secular frequency as a function of ion oscillation intensity can also be determined. This is done by using the "plane crossing" feature of Simion. This allows us to define a design procedure that can be used to optimize trap geometries for various purposes, for example, scanning from low to high mass as opposed to reverse scanning from high to low mass, and designing trap geometry for a particular scanning speed. One example of the design of a unique Paul trap optimized for high scanning speed will be given.

### Preliminary Data

The design procedure resulted in a 3D ion trap that had electrodes that looked somewhat different from a standard Paul trap. It was found that the center ring electrode could be made with straight sides and all curvature of the electrodes could be confined to the end caps. This could lead to easier machining of the trap electrodes. A standard Paul trap with no stretch has a constant secular frequency as the ions gain energy and approach the end-cap electrodes. It was found that in a stretched Paul trap with approximately 11% stretch, the secular frequency of the ions gradually increased by about 2.5% as the ions approached the end-caps. It was found that this degree of increase in the new 3D trap design could be made to match the commonly encountered stretched Paul trap, or it could be increased or decreased at will by changing the electrode design. Simulation data for a trap designed with approximately 6% increase in secular frequency as the ions go from the center of the trap to the end cap electrodes shows that good mass resolution can be maintained at higher scan speeds than those obtained for similar simulation data on the commonly encountered 11% stretch Paul trap.

**Transfer efficiency and timing performance measurements of multipole ion guides and ion wave guides constructed with planar technologies**

Albrecht Glasmachers<sup>1</sup>; Alexander Laue<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>; Michel Aliman<sup>2</sup>  
<sup>1</sup>University of Wuppertal, Wuppertal, GERMANY; <sup>2</sup>Carl Zeiss NTS GmbH, Oberkochen, GERMANY

**Novel Aspect:** First measuring results of multipole ion guides and ion wave guides produced with high precision planar technologies

**Introduction**

Mass spectrometry requires several process steps like ion generation, collection, cooling, fragmentation, selection and analysis which are often performed in specific stages. Between these stages the ions have to be transferred with high efficiency, high spatial and timing precision and with minimal ion energy spread. For these tasks structures with radial storage fields (ion funnels or linear multipoles) and axial transport fields (dc gradients for ion guides or moving potential wells for ion wave guides) have been developed in different variations using planar electronic technologies like printed circuits boards (PCB) or thick and thin film ceramics. The performances of these structures are evaluated by measurements and simulations.

**Methods**

Secondary ions generated on the surface of a target with e. g. an energy spread of more than 10 eV are transferred from a high vacuum (<10<sup>-6</sup> mbar) target area via electrostatic lenses into a multipole ion guide built by planar structures. There the ions are transferred by a dc gradient field while they are cooled by a damping gas (He). The ion intensities are measured using open Faraday cups with precise current measurements for the static operation of the ion guide and shielded Faraday cups combined with low noise charge amplifiers for the dynamic operation of the ion wave guide.

**Preliminary Data**

1. With a flexible PCB bent to a cylinder a multipole ion guide with an inner diameter of 16 mm and a length of 340 mm was built. Along the ion transfer axis it is divided into 36 equidistant segments. Eight planar metallic surfaces at the inner side of each segment produce the multipole rf storage field, while a superimposed dc potential per segment derived from a resistive divider chain generates the axial dc field gradient. The ion collection efficiency and the transfer efficiency within the ion guide are measured in dependency of operating parameters like ion mass, rf field strength, transfer field strength, and cooling gas pressure.

2. A cascaded quadrupole ion wave guide combined of a first part with 2 segments (rod diameter 5 mm, segment length 4 mm) and a second part with 11 segments (rod diameter 2 mm, segment length 4 mm) is fed with cooled ions from an ion guide. The ions are shifted by a 3-phase periodic pattern producing a potential well with a depth of a few Volts. The ion charge is measured by a low noise charge amplifier and recorded by an oscilloscope. As measurement results the influence of operational parameters like damping gas pressure, potential well depth and shape, and shifting speed are presented and compared to SIMION calculations.

**IonCCD™ for non-scanning sector-field instrument: from keV ion to image charge detection -- artifacts, performance and potential keV impact damage.**

Omar Hadjar<sup>1</sup>; Thomas Schlathoelter<sup>2</sup>; Stephen Davila<sup>3</sup>; Gottfried Kibelka<sup>1</sup>; Scott Kassar<sup>1</sup>; Chad Cameron<sup>1</sup>; Ken Kuhn<sup>1</sup>; Guido F. Verbeck<sup>3</sup>

<sup>1</sup>ITT | OI Analytical, Pelham, AL; <sup>2</sup>KVI - Atomic and Molecular Physics, Groningen, The Netherlands; <sup>3</sup>University of North Texas, Denton, TX

**Novel Aspect:** Novel 5-inch 2126-discrete microelectrodes for a new method of image charge detection in integration mode.

**Introduction**

Particle-surface interactions are very important processes, making physics practically impossible to apply without considering those interactions. For particle detection applications, the detection event is triggered by total or partial particle energy deposition upon impact with the detector. Common mass spectrometry ion detectors include Channeltrons and MCPs, which inherently destroy the particle upon measurement. FT-ICR and Orbitrap analyzers (R<sub>p</sub>>100.000) use image charge detectors that rely solely on the particle charge, hence detected ions are preserved for reuse. A third detector family is based on the rapidly emerging technology of pixilated detectors for charged particles, such as the IonCCD. This work focuses on the IonCCDs capability to detect image charge, covering instrument artifacts and performance.

**Methods**

The IonCCD is used as focal plane array detector in a sector-field instrument of Mattauch-Herzog geometry (MH-MS). When miniaturized, the MH-MS is best suited for low mass range applications (<100 u). Unlike the first two detector families, which most often operate in particle counting mode (time resolved detection), the IonCCD operates in an integration mode (charge integrator). In this case, dispersed ions neutralize on the electrode pixels for a well-defined time, known as the integration time. While the potential energy

of the detected ions is used for detection, the ion kinetic energy leads to ion-surface interaction, an artifact amplified at extremely low mass detection. Floating the IonCCD or operating it in higher magnetic fields can eliminate the artifact.

#### **Preliminary Data**

Experimental and theoretical data are used to discuss electronic-stopping induced mass spectra peak artifacts, their suppression, improving the tested instrument's performance, potential novel use of the detector, and potential damage induced from nuclear stopping. The artifact manifested in the mass spectra as distortion (negative peaks) due to keV ion impact-induced secondary electron emission is modeled and investigated experimentally using electronic-stopping power fingerprints. We demonstrate that the artifact increases linearly with ion impact velocity, and is dependent in an oscillatory fashion on ion nuclear charge. Both findings are in agreement with the electronic stopping of keV ions with the TiN surface of the IonCCD. 3D SIMION modeling suggests efficient peak artifact suppression by operating the IonCCD in a higher B-field (> 4000 G) and, less elegantly, by introducing a retarding field between the IonCCD and magnet face. The same model is used to enhance the performance of the instrument, confirming a dynamic mass range ( $M_{\max}/M_{\min}$ ) increase from 16 to 70.

Floating the IonCCD confirms the causal relationship between the observed artifact and secondary electron emission. It also allows, for the first time, observation of IonCCD sensitivity to image charge induced by glancing ions, which is modeled using reversal velocity analysis. This newly discovered capability, to be further investigated, could open new IonCCD horizons as a position-sensitive image-charge integrator in non-destructive measurements.

In order to investigate potential IonCCD damage upon keV ion impact through the nuclear stopping effect, surface characterization techniques are used. While atomic Force Microscopy (AFM) confirms the expected increase in surface roughness, X-ray Photoelectron Spectroscopy (XPS) shows no stoichiometry change due to implantation or preferential ion sputtering. The discoloration observed after extensive use is related to carbon layer formation in the roughened, irradiated pixel area. Nuclear stopping effects do not seem to affect the detector performance at practical doses.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 072, Thursday, Poster Hall

#### **Design of a Delayed Ion Injection Device to Improve the Detection Mass Range and the Sensitivity of FT-ICR MS.**

Myoung Choul Choi; Kyu Hwan Park ; Hyun Sik Kim  
*Korea Basic Science Institute, Ochang-Myun, SOUTH KOREA*

**Novel Aspect:** New optics and method to improve the TOF effect in the FTMS

#### **Introduction**

Most of Fourier transform ion cyclotron resonance mass spectrometers (FT-ICR MS) with an external source accumulate ions and transmit them to the ICR cell. During transmission through the ion guide, ions are dispersed in time because of mass discrimination effect (TOF effect). This effect often limits the detection mass range. To increase the simultaneous detection mass range and sensitivity, a delayed ion injection device has been designed in front of FT-ICR trap.

#### **Methods**

We've simulated a pulsed electric field gradient to narrow down the spatial distribution of ions. The pulsed gradient decelerates fast light ions more than slower heavy ions in a specific period of time. In this control, the field gradient shape, voltage, time duration can be optimized to focus the dispersed ions into the FT-ICR trap.

#### **Preliminary Data**

We have optimized the control parameters to minimize the TOF effect of ions in FT-ICR MS using SIMION program. The special distribution between the fastest mass (300 Da) and the slowest mass (2,500 Da) with the delayed ion injection device under the optimized conditions was improved several times. In this work, we present the optimal conditions of the delayed ion injection device.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 075, Thursday, Poster Hall

#### **Development of a portable mass spectrometer for operation at 1 Torr**

Feng Jin<sup>1</sup>; Guido F. Verbeck<sup>2</sup>; Glen P. Jackson<sup>1</sup>  
<sup>1</sup>Ohio University, Athens, OH; <sup>2</sup>University of North Texas, Denton, TX

**Novel Aspect:** This portable mass spectrometer can work up to 1 Torr with lower power requirement.

#### **Introduction**

In the early 1960s, a mass filter was built and tested by Eiber, which was shown to be capable of resolving O<sup>-</sup>, O<sub>2</sub><sup>+</sup>, and O<sub>3</sub><sup>-</sup> ions in an oxygen plasma at ~1 Torr. Eiber's filter accomplished this mass separation with a sinusoidal waveform of less than 5 Vpp. This demonstration remains the highest-pressure mass (not mobility) spectrometer tested to date. The vacuum along with low power requirement make it promising compared with other MS instrumentation. The immediate goals of this project are to reconstruct the mass filter using modern machining methods and to test/establish the mass filtration capabilities of the device using modern electronics and data-handling techniques. Potential applications include the health, environmental, defense and security sectors.

## Methods

Experiments are being performed on two home-made instruments; one with conventional electron ionization (EI) source, Einzel lens assembly and conversion dynode detector for testing in vacuum. The second configuration uses a glow discharge as an ion source and can operate from 10<sup>-4</sup> Torr to the pressure of the glow discharge. SOI-MEMS is used to reproduce the micro-positioned electrodes required for the Loeb-Eiber mass filter. Hard sphere collision model combined with SIMION 8.0 is used to rapidly simulate how groups of ions behave in electrostatic field at elevated (viscous) pressure.

## Preliminary Data

A significant number of SIMION simulations have been performed to understand the effects of operating parameters. The trajectory of ions is simulated under different operating conditions to assess the influence of kinetic energy and bath gas collisions on the m/z discrimination. Higher pressures of buffer gas cause more radial dispersion of the ions, as expected, but does not influence the mass filtering capability to a significant extent. Lower kinetic energies through the mass filter provide superior ion selectivity. Preliminary data show the ability to distinguish among different volatile organic vapors leaked into the glow discharge from an atmospheric sampling orifice. Vapors of acetone, methanol and ethanol are readily distinguished, albeit with lower than expected mass resolution. We will present the latest experimental and simulation results from our findings.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 078, Thursday, Poster Hall

### **Metrological characterization of a sensitive secondary ion mass spectrometer for electron microscopes to combine optical/structural and analytical imaging**

Alexander Laue<sup>1</sup>; Albrecht Glasmachers<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>; Michel Aliman<sup>2</sup>; Hubert Mantz<sup>2</sup>  
<sup>1</sup>University of Wuppertal, Wuppertal, GERMANY; <sup>2</sup>Carl Zeiss NTS GmbH, Oberkochen, GERMANY

**Novel Aspect:** First metrological characterization of an add-on secondary ion mass spectrometer for electron microscopes to combine optical/structural and analytical imaging.

#### Introduction

In modern natural sciences the combination of optical/structural and analytical imaging becomes more and more important. Today, electron microscopes use a focused electron beam for optical/structural imaging. For nano-scale manipulation and advanced structural imaging of surfaces a focused primary ion beam (FIB) is used. This primary ion beam produces secondary ions, which could be analyzed in a novel add-on secondary ion mass spectrometer (SIMS). This instrument must fulfill the hard requirements caused by the electron microscope environment (e.g. very limited space, broad kinetic energy distribution of the secondary ions and difficult vacuum conditions). It enables optical/structural and analytical imaging of the same target (spot) at the same time.

#### Methods

An add-on SIMS-device for an electron microscope was built, which incorporates four different stages for extracting, transferring, cooling and analyzing secondary ions. Every stage as well as the complete device was optimized, evaluated and metrologically characterized. The results are compared with numerical simulations.

For independent evaluation and characterization of single stages, different ionization methods are used:

- UV-Laser photo ionization of aromatic compounds for in-situ generation of ions
- Electron beam ionization of different sample gases to produce ions with a well defined kinetic energy distribution
- Focused primary ion beam to generate secondary ions of solid targets (real use scenario)

The influence of cooling gas flows and different electrical parameters, like ramping potentials, RF-frequencies and amplitudes, are evaluated.

#### Preliminary Data

The add-on secondary ion mass spectrometer was used with a Zeiss NVision Crossbeam electron microscope, equipped with a focused primary ion beam.

The extraction lens configuration of the SIMS-device, which incorporates also a differential pressure stage, was tested with different solid targets (silicon, silver, copper and lithium), surge potentials (-50 V ... -600 V) and damping gas flows (0 ... 50 sccm) to evaluate transfer efficiency and energy distributions of the secondary ions. The secondary ions are produced by a primary gallium ion beam with different primary kinetic energies (10 keV ... 30 keV) and different primary ion beam currents (100 pA up to 30 nA). The transfer efficiency and kinetic energy distribution of the secondary ions are compared with SIMION and SRIM numerical simulations.

The benching and transfer efficiency of the cooling section (axial segmented quadrupole linear ion trap made with planar technology for larger ion trapping cross section and an overall length of about 340 mm) as well as the energy distribution of different ions (with different cross sections) were evaluated by modifying electrical parameters (DC-Ramping: 0 ... -30 V; RF-Amplitude: 50 ... 250 V), damping gas flows (0 ... 50 sccm) and damping gases (nitrogen and helium). The measured results are compared with numerical simulations based on a hard sphere collision model in SIMION.

After the cooling-section the bunched ions are transferred through a second pressure stage incorporating a quadrupole ion waveguide (core diameter 1.8 mm), and pulsed into an electrical ion resonance cell, operating in Fourier transform mode. The waveguide frequency (1 ... 50 kHz), rf-amplitude (10 ... 50V), potential well (2 ... 5V) and pulse timing-parameter were modified. Pulse timing-parameters are critical, because a bad timing results in a significant loss of ions. Different pulse techniques and timings are evaluated for best transfer efficiency.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 083, Thursday, Poster Hall

### Lenses or No Lenses? A Study of Ion Transfer Efficiency at Interfaces in a Lens-less Triple Quadrupole MS

Felician Muntean; Roy Moeller  
Bruker Daltonics, Walnut Creek, CA

**Novel Aspect:** Provides experiments and analysis of lens-less coupling of rf ion guiding devices in a mass spectrometer.

#### Introduction

The sensitivity and robustness of triple quadrupole mass spectrometers make them the preferred work-horses of quantitative mass spectrometry today. The ion transfer between the several rf-based ion guiding and filtering devices: Q0, Q1, Q2, Q3 is critical to optimizing the sensitivity and robustness.

One traditional option is to use electrostatic lenses for collimating and refocusing ions while transferring from one "Q" to the next but lenses have the disadvantages of a cluttered instrument design, complex mass and energy dependent tuning, and susceptibility to contamination and instability.

Another option, discussed in this presentation is the lens-less direct coupling of the "Q" rf-devices, which has the advantages of simpler instrument design, straightforward tuning, and potential for better ion transfer.

#### Methods

Experimental data is taken on a Bruker triple quadrupole mass spectrometer. FC43 test compound molecules are ionized in an electron impact ion source, transferred through an RF ion guide Q0 into the first quadrupole Q1 where they are mass analyzed, transferred farther through the 180 degrees curved RF collision cell Q2 into the second mass analyzer Q3 and detected by a channeltron electron multiplier.

Simulations are performed using the SIMION 8.0 package and LUA programming for all components of this simulation. Collisions are modeled using a basic elastic collision, hard-sphere model.

#### Preliminary Data

Preliminary experiments characterize the ion transfer from an rf quadrupole collision cell into a quadrupole mass filter that are part of a triple quadrupole mass spectrometer. The collision cell is constructed with gas seals outside its rods, which allows it to be placed in close proximity to the mass filter, with no lens or aperture in between.

In the initial experiments, the effective cross section of the ion beam at the interface is reduced while monitoring the ion signal magnitude at m/z 131 at the detector in order to determine the condition of maximum transmission at the interface. The ion beam cross section is manipulated indirectly, by collision cooling and focusing in the collision cell. When the mass filter resolution is set to a wide resolution, flat-topped peak to approach 100% quad transmission, as the gas pressure in the collision cell is increased, the ion signal increases initially by about 10-20% beyond which it remains constant. At the same time, the resolved mass peak intensity keeps increasing significantly, a factor of three was observed at the maximum pressure investigated. This increase is a clear effect of reducing the ion beam size by collision focusing. The observation that the open resolution signal increases only 10-20% and then reaches a plateau while the beam size continues to be reduced through collision focusing indicates that we achieve 80-90% efficiency at this lens-less interface. The transfer efficiency reaches 100% with the aid of some collision focusing, by further increasing the operating pressure.

Further work that investigates the efficiency of similar lens-less interfaces in and out of mass analyzers and in terms of mass dependence, rf field parameters, separation distance at the interface, and pressure will be presented and discussed.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 086, Thursday, Poster Hall

### Ion trajectory calculations of ions entrained in neutral gas flow in the quadrupole field, utilizing superimposed flow fields and electric fields

Serguei Savtchenko<sup>1</sup>; Evgeny Makeev<sup>1</sup>; Jean-Francois Alary<sup>2</sup>; Sha Joshua Ye<sup>1</sup>  
<sup>1</sup>IONICS Mass Spec Group, Inc., Bolton, ON; <sup>2</sup>Isobarex Corp., Bolton, ON

**Novel Aspect:** First calculation of ion micromotion in damping gas flow fields, achieved by developing an interface between commercially available CFD and ion trajectory software

#### Introduction

Ion transmission through various pressure regions into the mass spectrometer between quadrupoles in RF-only mode needs to be optimised to achieve the high sensitivity requirements of modern mass spectrometers. Background flow coming into the chamber with

ions focuses them and also drags them downstream. A recent simulation approach was provided by Jugroot., et. al (J. Phys. D: Appl. Phys. 41 (2008)) using pseudo-potential formulation for the RF electrical field, averaging the effects of the RF field. However the amplitude of local motion of ions may not be small compared to the quadrupole field radius and often defines the exit angle of trajectory. The local (or micro) motion of ions can be best described by combining fluid dynamic simulation with ion trajectory calculation.

#### Methods

Here the flow field is pre calculated in FLUENT. The Spalart – Allmaras turbulent model is used for 3-D flow simulation with segregated solver. The 2-D unstructured mesh with adaption is used for the spatial discretisation. The processing includes velocities and density contours and profile building, drawing of the fluid particle tracks, etc.. For simulation of ion motion, the flow field is substituted in SIMION as a background gas flow. The simulations are initially done based on the Stokes law model for the interaction between ions and neutral background gas. The flow field is simplified and interpolated on the Simion calculation grid.

#### Preliminary Data

Detailed ion trajectories are presented for various pressure regimes, displaying the short time-scale ion motion superimposed upon the ion and flow velocities due to the combined flow and electric fields. Results show that the micromotion amplitude is sufficiently large to affect ion transmission in various pressure regions. It is shown that in higher pressure regimes ion trajectories are influenced by all those factors: electrical field, velocity damping and the flow pattern. Ions are focused to the centerline, and, for appropriate flow velocity and pressure combination, are at the same time forced to move ahead by the flow drag, effectively damping the small scale pulsations and focusing the ion beam. The axial component of the gradient for the pseudo potential in the fringe field regions is extremely important, and corresponds to the time averaged non-zero electric field which deflects ions away from the quadrupole entrance. The study shows that low energy ions are more likely to be reflected away if they enter the quadrupole off axis. The flow of gas with pressure about 1 torr may overcome this effect and drag ions through potential scattering regions.

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Poster: ThP04 - Instrumentation: New Developments in Mass Analyzers, poster number: 087, Thursday, Poster Hall

### Significant Improvements in Trapping Efficiency of Externally Injected Ions Using a Cylindrical Ion Trap with Increased Buffer Gas Pressure

Michael Goodwin; Mitch Wells

*FLIR Mass Spectrometry (Griffin), West Lafayette IN, 47906*

**Novel Aspect:** The increased trapping efficiency of a CIT at high pressures is more fully utilized by retuning focusing elements.

#### Introduction

Three dimensional ion traps suffer from poor trapping efficiency of externally generated ions. Previous theoretical studies predicted that trapping efficiency would increase significantly up to the Torr pressure range. However, experimental work in other groups demonstrated an optimum trapping efficiency of a few mTorr, with decreasing signal at higher pressures. The instruments in these experiments utilized electrostatic lensing to focus ions into the trap. The performance of electrostatic lenses degrades in the mTorr range due to scattering. As such, the previous experimental results represented a convolution of improved trapping efficiency and decreased transmission efficiency. If the focusing elements are adjusted accordingly, significant increases in signal can be observed at pressures higher than those previously reported.

#### Methods

Experiments were performed on a Griffin AI-MS instrument with an electrospray source and three stage vacuum system. The electrospray mixture was composed of dimethyl methyl phosphonate (DMMP), triethyl phosphate (TEP), tributyl phosphate (TBP), and tritoly phosphate (TTP). In the final stage an Einzel lens stack focuses ions into a cylindrical ion trap (CIT). The base pressure in the final stage was 1E-5 Torr, and helium was leaked into the chamber to a variable pressure. The DC voltages in the third stage were coarsely adjusted at each pressure for optimum signal. Simulations of the third vacuum stage were performed using SIMION 8.0 with a hard sphere collision model that mimicked helium.

#### Preliminary Data

Simulations were performed with ions of  $m/z$  125 injected into a CIT with 10 eV kinetic energy at various pressures up to 20 mTorr. Trapping efficiency increased linearly with pressure. However, simulations showed that the lens stack performance degraded at higher pressures. At 4E-4 Torr, ~95% of the ions were transmitted through the lenses into the CIT. At 10 mTorr with the same DC voltages, virtually no ions were injected into the trap due to scattering. When the voltages were re-tuned to account for increased collisions, the transmission efficiency could be returned to ~47% and a higher trapping efficiency was observed. An ~5x gain in the number of transmitted/trapped ions was observed for retuned lenses at 10 mTorr relative to normal tuning at 0.4 mTorr. Subsequent simulations utilized an octopole ion guide in place of the lenses. A gain of 19.3x in transmitted/trapped ions was observed for the octopole at 10 mTorr relative to the lens stack at 0.4 mTorr.

Experiments were performed on a Griffin AI-MS instrument with an electrosprayed mixture of DMMP, TEP, TBP and TTP. If the same lens voltages were utilized from 0.25 to 10.2 mTorr, the signal plateaued at 5 mTorr and decreased at higher pressures due to scattering in the lenses. When the DC voltages were re-tuned to pull the ions through the more frequent collisions at 10.2 mTorr, increases in signal were observed up to the highest pressure. The corresponding mass spectra show increases in signal at the highest pressure, with greater gains for higher  $m/z$  values. The signal was so intense at the higher pressure that space charge effects were noticeable. When the injection time was reduced for 10.2 mTorr, the resolution and measured  $m/z$  values at high and low pressures were similar.