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<th>Session</th>
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<td>10:30a</td>
<td>Field Optimization of Toroidal Ion Trap Mass Analysts using Toroidal Multipole</td>
<td>Jessica Higgs; Karl Warnick; Daniel Austin*</td>
<td>Brigham Young University, Provo, UT</td>
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<td>The Ohio State University, Columbus, OH</td>
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<td>Sandiya Garimella*; Yehia M. Ibrahim; Roza Wojcik; Ian K Webb; Richard D. Smith</td>
<td>Pacific Northwest National Laboratory, Richland, WA</td>
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<td>10:30a</td>
<td>Evaluation of kinetic energy distributions in atmospheric pressure ionization mass spectrometers (API-MS)</td>
<td>Marco Thinus*; Nils Rutenbach; Walter Wissdorf; Hendrik Kersten; Thorsten Benter</td>
<td>University of Wuppertal, Wuppertal, Germany</td>
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<td>Hendrik Kersten*; Chris Heintz; Walter Wissdorf; Thorsten Benter</td>
<td>University of Wuppertal, Wuppertal, Germany</td>
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<td>Fundamentals of Travelling Wave Ion Mobility Revisited (Smoothly Moving Waves)</td>
<td>Keith Richardson*; David Langridge; Kevin Giles</td>
<td>Waters Corporation, Wilsimso, United Kingdom</td>
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<td>10:30a</td>
<td>Pushing the mobility sensitivity, resolution and range with new electrode geometries in Trapped Ion Mobility Spectrometry</td>
<td>Alyssa Garabedian [1]; Juan Camilo Molano-Arevalo [1]; Kevin Jeanne Dit Fouque [1]; Mark E Ridgeway [2]; Melvin A Park [2]; Francisco Fernandez Lima* [1]</td>
<td>[1] Florida International University, Miami, FL; [2] Bruker Daltonics Inc., Billerica, MA</td>
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<td>10:30a</td>
<td>Dual Polarity Ion Confinement and Ion Mobility Separations in Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)</td>
<td>Isaac Kwame Attah*; IAN K. WEBB; Yehia M. Ibrahim; Christopher D. Chouinard; Gabe Nagy; Sandilya Garimella; Richard D. Smith</td>
<td>Pacific Northwest National Laboratory, Richland, WA</td>
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| WP 399 10:30am - 2:30pm | WP 399 Implementation of an Array of Traps and Ion Elevators in Structures of Lossless Ion Manipulations  
Aneesh Prabhakaran*; Sandilya Garimella; Randolph V. Norheim; Colby E. Schmeltferen; Spencer A. Prost; Cameron Giberson; Yehia M. Ibrahim; Richard D. Smith  
Pacific Northwest National Laboratory, Richland, WA  
Novel Aspect: Experimental demonstration of array of traps and elevator for complex ion manipulations with a multi-level SLIM device. |
| --- | --- |
| WP 400 10:30am - 2:30pm | Design and performance of a segmented ion trap with inductive detection used as a charged particle mass analyser  
Toby O. Rose¹, ²; Robert Appleby¹, ²; Keith Richardson³; Peter Nixon³; Martin Green³  
¹Cockcroft Institute, Daresbury, United Kingdom; ²University of Manchester, Manchester, United Kingdom; ³Waters Corporation, Wilmslow, United Kingdom  
Novel Aspect: We examine the capabilities and limitations of a new mass spectrometer with the potential for high resolution per unit time. |
| WP 410 10:30am - 2:30pm | Simulation Study of a U-shaped Mobility Analyzer for Multiple Operation Modes  
Keke Wang* [1]; Kent Gillig [2]; Xiaoxiang Zhang [1]; Long Chen [3]; Wenhuan Sun [1]  
¹Shanghai Jiaotong University Research laboratory (Shanghai) Co., Ltd., Shanghai, China; ²Academia Sinica, Taipei, Taiwan; ³Nanjing University of Aeronautics and Astronautics, Nanjing, China  
Novel Aspect: First high-resolution mobility filter based on cross-section, using counter flow mobility approach. And fast switching capability among three operation modes. |
| WP 467 10:30am - 2:30pm Wed, Jun 06 | Chemical kinetic and ion transport studies: Temperature dependence of ion mobility and its impact on cluster equilibria  
Duygu Erdogdu¹; Walter Wissdorf¹; Florian Stappert¹; Hendrik Kersten¹; Thorsten Benter¹; Bradley B. Schneider²; Tom Covey²  
¹Bergische Universität Wuppertal, Wuppertal, Germany; ²SCIEX, Concord, ON  
Novel Aspect: Numerical simulations of temperature dependent ion mobility, chemical dynamics and transport of ions through a DMS cell. |
| ThP 329 10:30am - 2:30pm | Operation and development of Ion-Mobility Orbitrap Mass Spectrometer  
Jacob W. McCabe*; Michael L. Poltash; Arthur Lagaronoky; David H. Russell  
Texas A&M University, College Station, TX  
Novel Aspect: This IM-orbitrap provides access to high-resolution IM-MS measurements of intact protein complexes while utilizing a first-of-its-kind interface to an Orbitrap. |
| ThP 462 10:30am - 2:30pm | Experimental Observation of the Effects of Translational and Rotational Electrode Misalignment on a Planar Linear Ion Trap Mass Spectrometer  
Yuan Tian; Joshua S McClellan; Trevor K Decker; Qinghao Wu; Abraham L De la Cruz Hernandez*; Aaron R Hawkins; Daniel E Austin  
Brigham Young University, Provo, UT  
Novel Aspect: First experimental results on the effects of electrode misalignment with multiple degrees of freedom in two-plane linear ion trap. |
| ThP 480 10:30am - 2:30pm | Development of a portable MALDI-TOF-MS for microbial identification  
Ko-Keng Chang* [1, 2]; Yi-Hong Cai [1]; Cheng-Chih Hsu [2]; Yi-Sheng Wang [1]  
¹Genomics Research Center, Academia Sinica, Taiwan; ²Chemistry Department, National Taiwan University, Taiwan  
Novel Aspect: The portable MALDI-TOF-MS is compact and low price, allowing wider variety of applications. |
| ThP 481 10:30am - 2:30pm | The fine-structure ion carpets for the transport of ions at atmospheric pressures  
Sergey Poteshin* [1]; Anna Burykina [2]  
¹National Research Nuclear University MEPhI, Moscow, Russian Federation; ²National Research Nuclear University MEPhI, Moscow, Russia  
Novel Aspect: Focusing system of ions at atmospheric pressure based on the fine-structure electrode with track pinch 10 µm. |
| ThP 513 10:30am - 2:30pm | Charge detection mass spectrometry of microparticles using printed circuit board electrode arrays  
Elaura L. Gustafson*; Halle V. Murray; Daniel E. Austin  
Brigham Young University, Provo, UT  
Novel Aspect: First evaluation of printed circuit board based charge detection for measuring the mass of individual microparticles. |
| ThP 519 10:30am - 2:30pm | Enhanced Resolution via Miniaturization of a Fourier Transform Electrostatic Linear Ion Trap Mass Spectrometer  
Joshua T. Johnson*; Kenneth W. Lee; Jay S. Bhanot; Scott A McLuckey  
Purdue University, West Lafayette, IN  
Novel Aspect: Resolution enhancement in a Fourier transform electrostatic linear ion trap with reduced axial dimensions. |
| ThP 521 10:30am - 2:30pm | Simulation of collisional interactions of background gas mixtures with trapped ions  
Thorsten Benter*; Walter Wissdorf; Marco Thinius; Hendrik Kersten  
Bergische Universität Wuppertal, Wuppertal, Germany  
Novel Aspect: Systematic investigations of the impact of the background gas composition on the ion dynamics in quadrupole ion traps. |
| ThP 523 10:30am - 2:30pm | Fundamentals of Cyclotron-Frequency FT-ICR MS  
Konstantin O. Nagornov* [1]; Anton N. Kozhinov [1]; Edith Nicol [2]; Yury O. Tsybin [1]  
¹Spectroswiss, Lausanne, Switzerland; ²Ecole Polytechnique, Palaiseau, France  
Novel Aspect: Performance characteristics and fundamentals insights of the cyclotron frequency generation and detection using ICR cells with narrow aperture detection electrodes. |
| ThP 526 10:30am - 2:30pm | Nonlinear Ion Trap Stability Diagram Mapping by Trajectory Harmonic Content  
Robert H Jackson* [1]; Stephen A Lammert* [2]  
¹Instrumental Design Physics, LLC, Littleton, MA; ²PerkinElmer Inc., American Fork, UT  
Novel Aspect: Mapping of separate r and z harmonic content over the stability region with initial condition dependence. |
MP 339 Fast two-laser submicron imaging mass spectrometry of small molecules

Time: MP 339 10:30am - 2:30pm  Mon, Jun 04
Authors: Jerome F Moore\textsuperscript{1}; Ernest K Lewis\textsuperscript{2}; Alexander Zinovev\textsuperscript{3}; Yang Cui (崔杨)\textsuperscript{4}
Institutes: \textsuperscript{1}Robot Nose, Lemont, IL; \textsuperscript{2}NASA Postdoctoral Program, Houston, TX; \textsuperscript{3}Argonne National Laboratory, Lemont, IL; \textsuperscript{4}Independent Consultant, San Jose, CA

Introduction: Imaging MS faces two fundamental challenges as the analysis voxel size decreases: 1. The analysis time for a given area increases by the inverse square of this size, and 2. The number of analytes decreases similarly. One opportunity for improving signal lies in the fact that the majority species are desorbed as neutral species. We previously demonstrated transmission geometry desorption directly into an ion funnel for improved collection efficiency. In the present work, we show a dramatic increase of ion yield in the source by using a vacuum ultraviolet (VUV) laser to ionize the predominantly neutral desorbed molecules.

Methods: Desorption is accomplished with a tripled Nd:YLF laser (349 nm, 1 microjoule), fiber optically coupled to a microscope with 10x objective mounted on a scanning stage. This stage has 0.1 micron precision and enables fast raster scan microprobing of the sample in transmission geometry. Desorption spot size is < 1 micron. Several microseconds after desorption, the VUV laser (157 nm, 1 millijoule) is fired and intercepts the desorbing molecules which are stagnating in the ion funnel. Ions from the funnel are transported with an RF hexapole to an oTOF for analysis and detection. Mass spectra are acquired on every shot at 500 Hz repetition, allowing for a fast analysis over a large area. SIMION was used to model the instrument.

Preliminary Data: We focus in the present work on analytes that are ionizable with one photon of 157 nm (7.87 eV) with minimal fragmentation: principally cholesterol, tryptophan, tyrosine, and suvorexant. As cholesterol is ubiquitous in animal tissues it provides a means of validating the technique for sectioned tissue samples especially at high spatial resolutions (subcellular). The amino acids are of interest in astromaterials studies for addressing questions on the origin of life. Suvorexant is an orexin receptor antagonist that has two conjugated systems that are ionizable at this photon energy. Results will be presented showing detection limit, linearity and images with determined mass and spatial resolution, effective contrast ratio and dynamic range. Comparison of direct desorbed (e.g. MALDI) data and two laser (e.g. MALDI-2, L2MS, LDPI, or postionization) data will be shown, in most cases there is an expected 5-10x increase in M+ signal with minimal induced fragmentation. Mass resolving power is limited by the energy spread into the compact oTOF to about 4000. This technique allows for an order of magnitude increase in signal, which makes the useful voxel size lower and allows for higher spatial resolution. The possibility to improve quantitation exists as well, since the large variation in ionization efficiency from a purely MALDI event is avoided, and saturation of the ionization event is possible.

Novel Aspect: Two laser fast imaging MS enables high throughput and high spatial resolution for screening tissues.

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MP 364 Field Optimization of Toroidal Ion Trap Mass Analyzers using Toroidal Multipoles

Time: MP 364 10:30am - 2:30pm  Mon, Jun 04
Authors: Jessica Higgs\textsuperscript{1}; Karl Warnick\textsuperscript{1}; Daniel Austin\textsuperscript{1}
Institutes: \textsuperscript{1}Brigham Young University, Provo, UT

Introduction: Toroidal ion traps show promise for miniaturized mass spectrometers, and have already been implemented in commercial portable GC-MS systems. However, because of the geometry of the trap, there remains a lack of understanding about the electric field and its effect on the motion of trapped ions. In all other types of ion traps, higher-order solutions to the Laplace equation (e.g., hexapole, octopole, dodecapole etc.) can be evaluated and adjusted to improve performance of the trap. However, in toroidal ion traps, these Cartesian solutions are not mathematically applicable. As an approach to this problem, solutions to the Laplace equation in a toroidal coordinate system can be used to characterize the electric potential distribution.

Methods: The symmetric 2nd order solution of the second kind, or toroidal quadrupole, was previously explored for an ion trap. Non-ideal features in the stability diagram (non-linear resonance lines, or black canyons, in which ions are lost) were similar to those for conventional ion traps with higher-order field contributions. To eliminate or reduce these non-ideal features, other toroidal solutions to the Laplace equation, including higher-order solutions, can be added to the toroidal quadrupole. Combinations of the toroidal quadrupole and other toroidal harmonics were calculated using MATLAB and input as geometry files into SIMION 8.1. Simulations of ion trapping were carried out in regions of the stability diagram where non-linear resonance ejection caused premature ejection of ions in the pure toroidal quadrupole.

Preliminary Data: The toroidal hexapole (T3) improves the stability diagram by reducing the jagged features at the stability apex and reducing the hexapole resonance line when the coefficient of the toroidal hexapole is in the range of 2.75. The beta(r) = ½ resonance line is eliminated by the coefficient of 1 or greater for the toroidal hexapole. The beta(r) = 2/3 resonance line is not present in the viewed voltage range when the toroidal hexapole coefficient is between 3.5 and 4.75, and the beta(z) + beta(r) = 1 resonance line becomes evident in this same range with the toroidal hexapole.
different gas loads. Trapped and thus makes it difficult to control ion load. Simion simulations were done to study the ion instability under conditions. The toroidal dipole (T1) changes the size of the stability diagram. The addition of a toroidal hexapole component to the toroidal quadrupole provides significant improvement in ion trapping by reducing the black canyons, and is expected to play an important role in optimizing the performance of all types of toroidal ion trap mass spectrometers. Mass analysis, with either boundary ejection or resonant ejection, has not been examined with these higher-order toroidal solutions, but we expect that other areas of trap performance may also improve, such as mass resolution.

**Novel Aspect:** Application of toroidal harmonics to optimize electric field in toroidal ion trap mass analyzers

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**MP 369 Development of Ion Carpet-Surface Induced Dissociation (SID) Devices for Simplified Tuning**

**Time:** MP 369 10:30am - 2:30pm Mon, Jun 04  
**Authors:** Alyssa Q. Stiving¹; Joshua D. Gilbert¹; Vicki H. Wysocki¹  
**Institutes:** ¹The Ohio State University, Columbus, OH

**Introduction:** SID has proven utility in the field of structural biology because of its ability to probe the topology of protein complexes by producing compact, charge symmetric fragments that are indicative of the original, native structure. As more structural biology groups become interested in this technique and request collaboration, improvements in ease of use are desired. With ten independent lenses, the current SID device design is not always straightforward to tune. Here, new SID devices are explored to alleviate these current challenges.

**Methods:** Simulations of various SID device designs were performed using SIMION 8.1.1. Installation was conducted using a Waters (Manchester, UK) Synapt G2 platform, placing the prototype device prior to the ion mobility cell. Device electrodes were machined in-house and the ion carpet printed circuit board was fabricated by Advanced Circuits (Aurora, CO). A ten-channel DC voltage supply (Aradara Technologies, Ardara, PA) provided voltages to the SID device lenses and ion carpet array. Standard protein complexes streptavidin, serum amyloid P component, and C-reactive protein (Sigma, St. Louis, MO) were prepared at ~10 µM in solutions of 100-200 mM ammonium acetate and ionized via nanoelectrospray.

**Preliminary Data:** Initial experiments were conducted using a cone electrode followed by an ion carpet consisting of 14 concentric electrodes resistively linked to one another. While this was met with some success, there were concerns with ion transmission efficiency when activation was not desired. Thus, a new design was machined utilizing a surface placed at a 45-degree angle from the ion path along with the “front bottom” electrode found in the original device nearly directly below it. This electrode pushes ions up towards the surface when a repulsive voltage is applied. Once ions collide with the surface, they are funneled back toward the original ion path with the ion carpet array, situated directly behind the surface. Success in both MS- and SID-modes has been shown for both devices with each being significantly easier to tune into SID-mode than the original ten-lens device. SID fragments were obtained within 5-10 minutes of initial tuning experiments, demonstrating more intuitive operation when compared with the original device that often takes a half day to tune from scratch. Well-studied protein complex systems allowed for confirmation of SID-like products. The energy at which ions collide with the surface can be easily adjusted by changing the potential between the trap cell exit and SID surface. While tuning has proven to be simpler, current experiments show SID product collection to be slightly diminished compared with the original ten-lens device. The use of more appropriate surface material as well as filling gaps in the ion path between the device and surrounding instrument parts is expected to improve fragment collection efficiency from initial experiments. Additional device designs such as incorporating an ion carpet in place of the last exit lens within the original ten-lens device are also being explored.

**Novel Aspect:** Results illustrate a new angled surface SID device design that provides an easy-to-tune alternative to existing ten-lens devices.

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**MP 373 Simulation study of ion stability of in-situ generated ions in a 3D ion trap under different gas load conditions**

**Time:** MP 373 10:30am - 2:30pm Mon, Jun 04  
**Authors:** Alexander Laue¹; Michel Aliman¹; Hin Yiu Chung¹; Valerie Derpmann¹; Ruediger Reuter¹  
**Institutes:** ¹Carl Zeiss SMT GmbH, Oberkochen, Germany

**Introduction:** 3D Ion Traps are commonly used for trapping and detection. In-situ ionization combined with a pulsed gas inlet system allows to build very compact and versatile devices. To avoid space charge effects ion load has to be controlled. One method is using the 3D Ion Trap as a combined mass filter and analyzer to suppress unwanted ions. This can be achieved by ion instability-mode (a- and q-parameters) or by resonant ion excitation, e.g. SWIFT. But collisions with residual gas or buffer-gas may prevent the ion to become instable due to the cooling effect: Unwanted ions are still trapped and thus makes it difficult to control ion load. Simion simulations were done to study the ion instability under different gas loads.
**Methods**: A complete simulation chain was built: In a first step time-dependent in-situ ion generation by electron impact was simulated using Simion and a Monte Carlo approach considering kinetic energy based electron cross sections. In a second step those generated ions were used to investigate ion dynamics. Different a- and q-parameter sets as well as different excitation signals (e.g. SWIFT) were used to study ion stability and instability under different residual gas and buffer gas loads. Simion and common hard sphere collision models were used. In a third step those results were evaluated by MATLAB programs and compared to theoretical considerations and models under ideal vacuum conditions.

**Preliminary Data**: Two different preliminary simulations studies were done to evaluate the simulation tool chain, code and models. First study was focused to get the simulation chain working: The simulation results are automatically passed to the next simulation or data processing tool and run without user interaction. Thus the setup is suited to run large numbers of simulations and parameter sweeps. The second study was done to evaluate and optimize the kinetic energy dependent cross section code for the in-situ ion generation simulations. The spatial and kinetic energy distributions were determined, showing good coincidence with theoretical considerations. Thus the simulation code is suitable for the main studies. Comparison values under ideal vacuum conditions were determined to compare those ideal results with the original simulation results to answer the following main questions of interest: What is the lifetime of ions inside the 3D Ion Trap by using ion instability mode (a- q-parameters) and resonant ion excitation? How ion stability regions (stability diagram) are shifted by residual gas and buffer gas collisions? Is there a time-dependent equilibrium of ion generation and ion loss? How ion instability is affected by modifying excitation signals and/or storage parameters (e.g. amplitude and frequency of the Radio-Frequency storage signal)?

**Novel Aspect**: Instability study with Simion of ions in a 3D Ion Trap under different gas load conditions

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**MP 376 Evaluation of kinetic energy distributions in atmospheric pressure ionization mass spectrometers (API-MS)**

**Time**: MP 376 10:30am - 2:30pm Mon, Jun 04

**Authors**: Marco Thinius¹; Nils Rutenbach¹; Walter Wissdorf¹; Hendrik Kersten¹; Thorsten Benter¹

**Institutes**: ¹University of Wuppertal, Wuppertal, Germany

**Introduction**: In API-MS the ion transfer stage is crucial for efficient sampling, ion beam shaping and ion transport from atmospheric pressure into the high vacuum recipient of the mass analyzer. Even though ions are driven towards the analyzer by electric fields over the entire length of the transfer stage, only acceleration under low-collision or collision-free conditions leads to an increase of kinetic energy. The kinetic energy distribution of the ions becomes important during the transfer into the mass analyzer. This contribution focuses on the characterization of ion transfer stages in commercial mass spectrometers with regard to the ion kinetic energy distribution and the impact of acceleration voltages in different pressure regions of the transfer stage.

**Methods**: Kinetic energy distribution measurements are performed with Bruker ion trap mass spectrometers (esquire6000, HCT plus, amazon Speed ETD). For stable and reproducible ion generation the Bruker Apollo ESI source is used. Kinetic energy distributions are determined by successively increasing the potential difference between the ion transfer stage and the ion trap entrance so that only ions with a sufficiently high kinetic energy can enter the ion trap. The derivative of the kinetic energy dependent ion chromatogram yields the kinetic energy distribution. Absolute ion currents exiting the ion transfer stage are measured with a Keithley Instruments 610C Solid State Electrometer. SIMION simulations are used for qualitative studies of collision induced changes of the kinetic energy of ions.

**Preliminary Data**: The kinetic energy distribution of ions exiting the ion transfer stage is determined from direct ion current measurements and ion chromatograms by applying adjustable deceleration potentials between transfer stage and detector/mass analyzer. Ion currents are on the order of pico-Ampere/s for standard transfer preset values. The center and width of the kinetic energy distribution as well as the maximum ion current is strongly dependent on the acceleration potentials applied in the transfer stage. The respective impact on the kinetic energy distribution depends further on the local pressure prevailing. Strong acceleration in intermediate pressure regimes can result in non-intuitive behavior, as the gained kinetic energy is partly redistributed into the background gas. Simulations using SIMION with a hard sphere collision model show that the kinetic energy distribution of an accelerated ion population is significantly altered by collisions with the background gas. To our surprise a shift of the kinetic energy distribution is observed when changing the ESI voltage using the esquire and HCT instruments. Performing identical experiments with the amaZon instrument, no such impact is noticed. The main difference between the instruments is the API interface, which consists either of a capillary-skimmer system (esquire and HCT), or a dual-funnel stage (amaZon). In contrast to the capillary-skimmer setup the funnels are operated with rather strong RF fields used for ion focusing. Thus, in addition to ion beam formation the funnel stage forces strong declustering reactions by RF heating. It is speculated that this results in efficient evaporation of nano-droplets which otherwise (capillary/skimmer setup) may reach the deep vacuum stages of the instrument. The change of the ion kinetic energy distribution with different ESI voltages is thus attributed mainly to the existence of nano-droplets in the transfer stage rather than to changing droplet size distributions in the ESI process.
**Novel Aspect**: Characterization of electric field effects and potential ion heating in different TW-based ion guides.

**MP 382 Simulation of ion trajectories in an electrostatic Bessel-box type energy filter**

**Time**: MP 382 10:30am - 2:30pm  
**Mon, Jun 04**

**Authors**: Hendrik Kersten¹; Chris Heintz¹; Walter Wissdorf¹; Thorsten Benter¹

**Institutes**: ¹University of Wuppertal, Wuppertal, Germany

**Introduction**: The Bessel-box is a kinetic energy filter, first introduced in 1976 by Allen et al. Herein a beam of charged particles with a certain kinetic energy distribution enters a cylindrical electrode through a pinhole entrance. The beam is deflected from its straight path through the cylinder by a small center electrode. Consequently, only particles with a kinetic energy matching the forces of the electrical field inside the box follow a trajectory around the center plate and can leave the Bessel-box through a second pinhole in the exit electrode. This energy filter is used, e.g., by Hiden Analytical, upstream of the quadrupole analyzer. We present numerical results on the transmission and filter characteristics of this particular Bessel-box.

**Methods**: The geometry of the Bessel-box under investigation was taken from the user’s manual of the HPR60 quadrupole mass spectrometer from Hiden Analytical Ltd. Electrical fields and corresponding ion trajectories were simulated with Simion 8.1. Custom Lua scripts and python code allowed for automated simulation processing, data visualization and analysis. Each simulation started with an initial ion population of 10 000 singly charged particles with a mass of 3 Da and an evenly distributed initial kinetic energy ranging from 0 to 10 eV.
**Preliminary Data:** The HPR60 uses an axially aligned Bessel-box between the electron ionization source and the quadrupole analyzer. Essentially the instrument allows two voltages of this device to be adjusted: The endcaps in the range of ± 90 V, both at the same value, and the cylindrical electrode in the range of ± 10 V. The center plate is directly connected to the cylinder voltage. In particular, we were interested in the characteristic kinetic energy filter bandwidth, the filter range and the transmission efficiency of this device. First simulations showed that the endcap voltage largely determines the filter energy bandwidth, whereas the cylinder voltage has virtually no impact. For endcap settings between -50 and + 5 V our results suggest a minimum and maximum filter width of 0.5 eV and 3.5 eV, respectively. The cylinder voltage is responsible for the mean value of the transmitted ion energy, whereas the effect of the endcap potential is negligible in this case. For the possible settings of this particular device we found transmitted energy distributions around mean values of 0.8 up to 9.6 eV. To determine transmission efficiencies the total number of transmitted ions in a small energy range was related to the total number of generated ions within this range. Our simulations suggest a maximum transmission efficiency through the Bessel-box of 50%. The parameter mainly responsible for the transmission is again the endcap voltage, as was the case for the bandwidth. In several simulations we found rather diverging trajectories for ions exiting the Bessel-box. In upcoming simulations we will model the capability of the subsequent lens structure to capture and transfer the ions into the analyzer.

**Novel Aspect:** Simulation of a Bessel-box energy filter: filter width, filter range and transmission efficiencies

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**MP 392 Fundamentals of Travelling Wave Ion Mobility Revisited (Smoothly Moving Waves)**

**Time:** MP 392 10:30am - 2:30pm Mon, Jun 04  
**Authors:** Keith Richardson; David Langridge; Kevin Giles  
**Institutes:** Waters Corporation, Wilmslow, United Kingdom

**Introduction:** Travelling Wave Ion Mobility (TWIM) has been in use since around 2004. Ions are separated by a series of DC waves which overtake them and push them through a gas filled RF ion guide. Less mobile species are overtaken more frequently than highly mobile species, producing a mobility dependent average velocity. The relationship of average velocity to travelling wave parameters and mobility is complicated, so TWIM instruments are usually calibrated using drift tube measurements. There is, however, no fundamental obstacle to making direct mobility measurements in TWIM devices. We give a new theoretical treatment of TWIM, deriving an exact expression for smoothly moving sinusoidal waves as well as demonstrating that anharmonic corrections and velocity relaxation effects can be included systematically.

**Methods:** A generalised and simplified expression for the average velocity of an ideal ion of mobility K in a TWIM device utilising an arbitrary waveform E(x,t) is derived. This expression is valid for asymmetric waveforms. The average ion velocity can be expanded in powers of K, with odd powers of K vanishing for symmetric waves. We give the exact result for a sinusoidal wave (a good approximation to the waveform in commercial TWIM mass spectrometers). This approximation is improved by systematically incorporating anharmonic corrections. We further generalise our results, treating velocity relaxation effects (arising from finite ion acceleration times) perturbatively. SIMION simulations are used to examine whether these results remain valid when diffusion is incorporated in our model.

**Preliminary Data:** The average ion velocity for an ideal ion of mobility K in a smoothly moving sinusoidal TWIM device with wavelength λ, wave velocity v and amplitude V_0 is v(1 - ω_0^2), where ω_0=ω_0(1 - γ^2) and the critical dimensionless parameter γ=2π K V_0 / (v λ). For γ<1, conditions are mobility separating, while for γ>1 ions surf on the wave without experiencing roll-overs. Under typical conditions, anharmonic corrections change the average velocity by up to about 5%. Velocity relaxation effects introduce some mass-to-charge dependence into the average ion velocity. The size of these effects is governed by the dimensionless parameter α, which is the ratio of the relaxation time to the travelling wave period. Velocity relaxation induces shifts in measured collisional cross sections (CCS) of up to about 1% for small molecules and peptides under standard conditions. These effects can be removed by taking relaxation into account explicitly during the calibration process. Larger changes are observed for compounds such as native protein complexes which have unusually high mass-to-charge ratios. We find that conditions already reported to improve experimental CCS measurement accuracy for these molecules also tend to minimise simulated calibration errors resulting from relaxation effects. Finally, we show that, under typical conditions, diffusion is not strongly coupled to average axial ion motion. We discuss the prospect of uncalibrated smoothly moving travelling wave experiments as well as considering how relevant our results are to current commercial systems employing stepped (digital) travelling waves.

**Novel Aspect:** New results in TWIM theory, promising improved calibration accuracy and raising the possibility of uncalibrated CCS measurements.

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**Tue Oral - Pushing the mobility sensitivity, resolution and range with new electrode geometries in Trapped Ion Mobility Spectrometry**

**Time:** Ballroom 20A TOB am 09:10 9:10am - 9:30am Tue, Jun 05
Introduction: With the advent of trapped ion mobility spectrometry in 2011, a major transformation is occurring in the way mobility separations are performed, due to the high resolving power (R=150-250, with reported up to 400), high sensitivity (ppt level) and it's recently coupling with high and ultrahigh resolution mass analyzers (TOF and FT-ICR MS). In TIMS, the mobility separation is currently limited by the trapping and elution strategies, since ions can undergo almost infinite drift lengths (gas velocity x trapping time). In the present work, we introduce a new mobility cell design, with enhanced sensitivity, resolution and range. Theoretical and experimental data will be presented to describe the main parameters and performance of the new cell design.

Methods: In the new design, the TIMS analyzer section is typically comprised of 20-25 PC boards, electrically insulated, and each board contains two pairs of opposite electrodes at the same state (voltage and radiofrequency phase). The shape of the electrode was varied from concave to convex, leading to higher penetration pseudopotentials. The performance of the new cell was evaluated in an in-house built TIMS-TOF MS platform for a variety of native proteins, intrinsically disordered proteins, antibodies, and biomolecular complexes: HMGA2, BSA, CLAMP, E. Coli Topoisomerase I, Topoisomerase1-DNA; IgG, and GroEL-.... Ion dynamic simulations were performed in SIMION using an elastic hard sphere scattering model.

Preliminary Data: The pursuit for new electrode TIMS geometries focuses on the possibility to apply higher penetration radial fields and to increase the trapping volume, leading to larger mobility ranges and higher sensitivity. SIMION simulations showed similar ion behavior despite the electrode shape, but with smaller RF amplitudes require to trap ions in the convex geometry; the RF amplitude can be a limiting factor during TIMS due to potential electric discharges at high values. A dependence on the mobility range with the trapping frequency was observed and further verified experimentally. Optimal conditions were found when using high rf (~2MHz, Vpp = 150-300) for low m/z = 100 – 900 (or high mobility) and low rf (450 kHz, Vpp = 200-280) for high m/z = 600 – 15k (or low mobility). Experimental results confirmed the higher sensitivity (low ppt) and better trapping across a larger mobility (and mass) range. A resolving power over 150 was routinely observed with low resolution scan rate (Sr= 0.3 V/ms) for high mass scans. The performance characteristics were evaluated using a Tuning Mix standard solution (n=1-3) and CsCl cluster ions (m/z up to 10k). The mobility analysis of native proteins, protein-DNA and protein-protein complexes was successfully extended to the m/z 500-15k range over the mobility range 0.3-1.8 cm V s⁻¹. This allow the observation of the following species during native conditions: HMGA2 (MW 12 kDa), BSA (MW 66 kDa), CLAMP (MW 88 kDa), Topo I (MW 97 kDa); HMGA2-DNA (MW 27kDa); Topo1-DNA (MW 114kDa); IgG (MW 150 kDa), and GroEL (MW 58kDa). The influence of the solution-gas-phase transition on the observation of protein oligomers (e.g., pre-formed vs formed during nESI) was evaluated using the CLAMP WT and mutant proteins; results show that gas-phase distributions are likely a replica of the solution oligomeric distributions for the conditions studied.

Novel Aspect: New electrode geometry in TIMS with high mobility resolution, sensitivity (low ppt) and wide mass range (up to MDa)
investigated by combined SIMION and SIMAX software. National Instrument modules were used for ionization, trapping voltage control, and induced signal detection. Low noise homemade preamplifier was used for induced voltage detection.

**Preliminary Data:** Among four electrode Kingdon trap geometries giving trapping fields with quadratic dependences of electric potentials on one of the coordinates and satisfying Laplace equation the geometry with fused electrode pairs was chosen. The trap with such geometry electrodes was found to be less sensitive to surface imperfections and truncation of the electrodes. Many variants of the trap were manufactured: by regular machining method and by 3D printing. Different metal powder was used in case of 3D printing: stainless steel for selective Laser Sintering and Inkjet Metal Printing and silver in the case of microcasting. Two types of the trap were manufactured and tested experimentally. In the first variant ions are introduced into the trap from outside in the way similar to what is used in the Orbitrap. This trap has two separated external electrodes for induced current detection. In the second variant of the trap ions are introduced to the center of the trap or produced just inside the trap. Their detection is performed by SWEEP excitation of their motion and detection of the voltage induced by excited ions (like in FT ICR). To do this two external (excitation) electrodes are added to the trap. Initial evaluations of different traps performances will be given.


**Novel Aspect:** FT mass spectrometer based on multiple (fused) electrodes harmonized electrostatic trap of Kingdon type is demonstrated.

**Wed Oral - Ultrahigh Resolving Power Ion Isolation by 21 T FT-ICR MS**

**Time:** Hall D  WOA pm 02:50 - 2:50pm - 3:10pm  Wed, Jun 06

**Authors:** DONALD F. SMITH1; Greg T. Blakney; Steve C. Beu2; Christopher L. Hendrickson1, 3

**Institutes:** 1National High Magnetic Field Laboratory, Tallahassee, FL; 2S. C. Beu Consulting, Austin, Texas; 3Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL

**Introduction:** Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry provides the highest achievable mass resolving power and mass accuracy of any mass analyzer. Mass resolving power improves linearly, while mass accuracy and dynamic range improve quadratically with increasing magnetic field strength. In addition, the ion isolation mass resolving power achievable by stored waveform inverse Fourier transform (SWIFT) also increases linearly with magnetic field strength. Here, we report ion isolation mass resolving power of up to 170,000 (@ m/z 597), for isolation of two ions that differ by 3.4 mDa (C3 vs. SH4), which is the highest ion isolation mass resolution achieved to date. Computer simulations are used to determine the fundamental performance limit.

**Methods:** Isolation experiments were performed on the NHMFL 21 T FT-ICR mass spectrometer equipped with a dynamically harmonized ICR cell (DHC). Canadian bitumen was analyzed by negative ion microelectrospray at 250 µg/mL in 50:50 toluene/methanol with 1% NH4OH added to aid deprotonation. Prior to SWIFT isolation, an ion trap isolation (5-20 Th) was performed, centered on the ion m/z of interest. A Predator data station was used for SWIFT isolation, excitation, and detection. Simulations were performed with SIMION (Version 8.1, Scientific Instrument Services, Ringoes, NJ) running on a homebuilt 3.00 GHz AMD Phenom II Quad-Core PC with 16 GB DDR3 ram.

**Preliminary Data:** SWIFT isolation resolving power scales linearly with magnetic field strength and with the duration of the SWIFT waveform. Isolation resolution is reduced by a poor trapping electric field, magnetic field inhomogeneity, or voltage imbalance in the SWIFT waveform. The NHMFL 21 T has been designed to minimize these limitations. The dynamically harmonized cell (DHC) generates an azimuthally averaged trapping electric field that approaches ideal over the entire cell volume. The NHMFL 21 T magnet has a spatial magnetic field inhomogeneity of less than 5 ppm over a 60x100 mm cylinder. The cyclotron frequency of ions at m/z 515 changes by less than 1 Hz when excited from 30-98% cell radius (single frequency excitation). An isolation resolving power > 150,000 is required to individually isolate two ions with a mass difference of 3.4 mDa at m/z 515. The frequency difference is ~4 Hz, well within the frequency deviation during excitation. A 16 MB SWIFT excitation (0.84 s excitation duration) was used to isolate each ion, with an isolation efficiency of 50%. The initial ion trap isolation yielded 1,140 ions over the 5 Th isolation width. The broadband mass spectrum contains over 50,000 peaks, to which 36,000 can be assigned a unique elemental composition. At m/z 597, an isolation resolving power of 175,000 is required to isolate ions with a mass difference of 3.4 mDa. A 32 MB SWIFT excitation (1.68 s) was used to isolate each ion, with an isolation efficiency of ~17%. Perspectives for single ion tandem MS of complex mixtures will be discussed, as well as application to online LC-MS/MS for biological applications.
Novel Aspect: SWIFT ion isolation resolving power > 170,000 by 21 T FT-ICR MS.

Wed Oral - Towards increasing the performance of FTICR-MS with signal detection at frequency multiples: signal theory and numerical study

Time: Hall D WOA pm 03:10 3:10pm - 3:30pm Wed, Jun 06
Authors: Qinghao Wu1; Mikhail Gorshkov2; JARED B. SHAW3; Ljiljana Pasa Tolic3
Institutes: 1Pacific Northwest National Laboratory, Richland; 2V.L. Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russia; 3PNNL, Richland, WA

Introduction: Further increasing acquisition rate in high resolution mass spectra is needed in FTICR-MS to meet the challenges of intact protein characterization in top-down proteomic applications, complex mixture characterization and mass spectrometry imaging. Detection of signals at cyclotron frequency multiples using multi-electrode ion traps, so-called nX-ICR cells, allows for acquisition of high resolution mass spectra at significantly increased acquisition speed. However, multiple detection scheme also requires trapping ions at high orbital radii for improved sensitivity. Herein, we present a theoretical ground that reveals the factors affecting signal-to-noise ratio, and intensity of undesired harmonic peaks thus laying the ground for further improvements of the nX-ICR cell technology.

Methods: The theory is based on the calculation of the image current acquired using two types of detection electrodes inter-connections in the nX-ICR cell and provides a relationship between nX-ICR cell parameters and the signal-to-noise ratios (S/N) for both connection types. These parameters include detection circuit input resistance, R, bandwidth, Δf, magnetic field, B, ion mass, m, ion charge, q, relative orbital radius, η, relative radius of the electrode, η2, and electrode number M. Magnetron motion was further introduced into the theory by adding magnetron radius, η3. The developed theory was integrated into the SIMION-based models to characterize of the effect of the electrode shape and operational parameters on the resulting mass spectra.

Preliminary Data: Based on the theory, we found that the S/N at the main harmonic peaks has simple relationships with several parameters, such as η2, T, B, m, and q. Other four parameters, including η1, η2, η3, and M, affect differently the S/N: η1 could dramatically increase the S/N; η2 can be optimized for achieving the highest S/N; larger number of electrodes (M) reduces the S/N at low orbital radius and increases S/N at high orbital radius; and η3 has no significant impact on the S/N. The relationship between peak intensities of main harmonic peaks in type II connection was studied using the ratio between the intensities of the first two major harmonic peaks, S/M2/S/M2 with 16 electrode cell design, the results showed that this ratio is decreasing with η1/(1-η2) and is increasing with η2. Further, S/M2/S/M2 is increasing with M, and η3 has no significant effect on this ratio. The lower frequency harmonic peaks were characterized by the ratio, S/M2/S/M2, between the intensity of harmonic peaks of n = M2 and M/2. For 16 electrodes, this ratio is mainly affected by η3 and is slightly increasing with η1. In addition, it can be further increased by reducing the electrode number M. Comparing different models generated by SIMION, we found that the reciprocity has limited impact on the peak intensity and do not have a significant impact on the S/M2/S/M2 and S/M2/S/M2 for the 16 detection electrodes detection scheme. The peak intensities in rod electrodes and segmented cylindrical electrodes at the 8th harmonic are 2.1 and 2.8 folds increase than that in theoretical sphere electrodes, respectively. The shape of detection electrodes also has an impact on the S/M2/S/M2, but does not have a significant impact on S/M2/S/M2.

Novel Aspect: A comprehensive theory of the spectra acquired using nX-ICR cell with different types of multi-electrode detection scheme was proposed.

WP 392 Dual Polarity Ion Confinement and Ion Mobility Separations in Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)

Time: WP 392 10:30am - 2:30pm Wed, Jun 06
Authors: Isaac Kwame Attah1; IAN K. WEBB1; Yehia M. Ibrahim1; Christopher D. Chouinard1; Gabe Nagy1; Sandilya Garimella1; Richard D. Smith1
Institutes: 1Pacific Northwest National Laboratory, Richland, WA

Introduction: Structures for Lossless Ion Manipulations (SLIM) have been rapidly gaining prominence for applications where ultra-high resolution Ion Mobility (IM) separations are desired to provide performance features and information unattainable using the currently available IM platforms. Although most routine analyses are done in either positive or negative polarity modes, there are significant benefits to both, potentially making them highly complementary if performed simultaneously. In the effort to develop a robust dual polarity IM platform, we explored an evaluation of a novel SLIM platform developed to perform simultaneous cationic and anionic IM separations (i.e. without requiring polarity switching).

Methods: These studies were conducted using a home-built nanoESI-SLIM IM platform coupled to an Agilent TOF-MS. The traveling wave SLIM device was fabricated using photolithography. Ions were produced by a nanoelectrospray ionization into an interface incorporating an ion funnel, which were then pulsed into the SLIM device using the conductance limiting plate of the funnel as a gate. Ion transmission efficiency performance of the SLIM device is assessed
by quantitative ion current measurements at different locations in SLIM. Ions exiting the SLIM device were also analyzed using the mass spectrometer to assess the ion transmission as a function of m/z. The experiments were performed using Agilent low concentration tune mix.

**Preliminary Data:** Initially, a continuous ion beam of a chosen polarity was injected into the SLIM device from a travelling wave (TW) based ion funnel. Ion current measurement were made at the entrance of the SLIM device using a wire probe inserted in-between the SLIM surfaces. Ion current measurements were then performed at several points along a 0.9 m long path length, which has four 90° turns. Separate ion current measurements suggests lossless ion transmission through the SLIM device for either positive or negative ions under the same conditions. To achieve the dual polarity operation the static (DC) potentials applied to the ‘guard’ electrodes used in earlier SLIM were replaced with dynamic voltage (RF) potentials to provide lateral confinement of the ions. The optimum RF conditions required in this new SLIM device to successfully confine and transmit ions of both polarities were investigated using a tunable RF generator, and the optimized values were found to be approximately 400 Vpp, 0.5 MHz. The TW and RF parameters used for the SLIM were 30 Vpp, 0.2 MHz and 320 Vpp, 0.8 MHz respectively. SIMION simulations were performed to gain more understanding of the experimental observations, revealing that the nature of the TW profile presents a potential minima at the opposite ends of the voltage wave for the respective ion polarity as the wave transverses the segmented TW electrodes, thus enabling efficient ion transport, without requiring a TW polarity change.

**Novel Aspect:** A SLIM device capable of performing simultaneous positive and negative ion IM separations in the same ion path.

**WP 399 Implementation of an Array of Traps and Ion Elevators in Structures of Lossless Ion Manipulations**

**Time:** WP 399 10:30am - 2:30pm Wed, Jun 06

**Authors:** Aneesh Prabhakaran; Sandilya Garimella; Randolph V. Norheim; Colby E. Schimelfenig; Spencer A. Prost; Cameron Giberson; Yehia M. Ibrahim; Richard D. Smith

**Institutes:** Pacific Northwest National Laboratory, Richland, WA

**Introduction:** Previous demonstrations of SLIM technology have enabled ion mobility (IM)-MS measurements with extended path lengths, complex manipulations of ion peaks, switching, ion elevators between two levels and compression ratio ion mobility programming (CRIMP). Such concepts provide a basis implementation of multi-level of SLIM utilizing traveling waves (TW) for providing unprecedented IM resolution and peak capacity. The flexibility of TW SLIM allows for precisely separated ion species to be selected and redirect to another path. Subsequently, selected ions can be accumulated a designated trap in an “arrays of traps” in the SLIM device, to enrich selected mobilities, perform ion chemistry, and other manipulations.

**Methods:** The array of traps was designed in a SLIM with 6,5 configuration (6 RF electrode strips and 5 interleaved DC TW electrodes) with DC TW electrode size of 1mm. Pulsed ions were injected into a 4 meter long serpentine path from an Ion Funnel Trap. Two TW were used, one in the serpentine path for ion mobility separation and another TW in the array of traps for optimum trapping. Those mobility separated ions in the serpentine path were then directed into separate traps using a DC switch/tee arrangement. Longer path for ion mobility separation were achieved by introducing the elevator concept, where there are several SLIM levels in parallel and between which ions can be efficiently transported.

**Preliminary Data:** An initial evaluation of the array of traps concept was made using a single level module with ion packets introduced in 324 µs pulses from an ion funnel trap into the SLIM incorporating an array of 32 traps. The trapping capability was demonstrated by accumulation of tune mix m/z 622, 922, 1222 and 1522 ions separately in different traps and releasing them after a selected accumulation time (162 millisecond). No loss of ions was observed during the trapping and releasing process. Also, it was shown that the ions could be continually accumulated up to the charge capacity of the SLIM traps. To enable high selectivity for a narrow range of mobilities to be trapped, ions were first separated in a multilevel SLIM. To enable multi-level SLIM ion elevator designs were refined using SIMION simulations, to achieve lossless ion movement and separation. The ions were elevated to the next level by applying appropriate potentials to selected electrodes so as to direct ions into an orifice separating the two SLIM levels. The specific electrode arrangements and TW conditions that enabled lossless ion transport from one level of SLIM to another were studied and optimized. SLIM designs with ion elevators and multiple levels were assembled with one of the levels dedicated to ion switching and accumulation of selected species. The design efficient transport of ions from one level to the next and accumulation of selected species with very high specificity. Performance of the multi-level SLIM was evaluated using variety of samples.

**Novel Aspect:** Experimental demonstration of array of traps and elevator for complex ion manipulations with a multi-level SLIM device.

**WP 400 Design and performance of a segmented ion trap with inductive detection used as a charged particle mass analyser**
**Introduction**: Fourier transform (FT) mass spectrometers achieve high resolution using relatively long transient times. This can limit hybridisation with other separation techniques. By contrast, time-of-flight (ToF) mass spectrometers have relatively short flight times and, generally, lower resolution. We propose a novel mass analyser comprised of an ion trap constructed from a series of pairs of concentric ring electrodes, utilising inductive ion detection with the potential for the short transient of ToF devices, and the high resolution of FT devices. Here we describe the design and theoretical performance of the mass analyser, detection electronics and use of a Bayesian signal processing algorithm.

**Methods**: SIMION 8.1 ion optical modelling software was used to analyse and record ion trajectories, and to simulate and record the differential induced signal on two central electrodes. The response and noise characteristics of the signal amplification electronics are simulated. The signal is then processed by a Bayesian forward-fitting algorithm, to explore the performance of the device.

**Preliminary Data**: We find that the electric potential is accurate enough to support stable circular orbits when generated by a series of concentric rings, and the perturbations due to the addition of detector electrodes can be accounted for. The phase space properties of the ions are investigated, and the initial distributions are modified to make use of natural focussing at the central plane of the device. In the ideal scenario, where space charge effects, amplification distortion, electronic noise are all negligible, the resolution of this device can be as high as 250,000 in a 3ms transient, scaling approximately proportional to the square root of the trapping time. When sources of error are introduced at realistic levels, the resolution is limited by electronic noise at the lower limit of detection. Prospects for further reducing the electronic noise, and thereby increasing the instrument resolution, are discussed.

**Novel Aspect**: We examine the capabilities and limitations of a new mass spectrometer with the potential for high resolution per unit time.

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**WP 410 Simulation Study of a U-shaped Mobility Analyzer for Multiple Operation Modes**

**Time**: WP 410 10:30am - 2:30pm Wed, Jun 06

**Authors**: Keke Wang; Kent Gillig; Xiaoyang Zhang; Long Chen; Wenjian Sun

**Institutes**: Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China; Academia Sinica, Taipei, Taiwan; Nanjing University of Aeronautics and Astronautics, Nanjing, China

**Introduction**: A U-shaped mobility analyzer (UMA) was developed as a powerful ion mobility analyzer using counter flow method to achieve very high resolution for both targeted and non-targeted mobility analysis. UMA has two parallel 2-dimensional drift channels in which electric field is opposite to the gas flow direction which is perpendicular to the original ion axis. Benefiting from its U-shape and planar structure, the UMA can be operated in three different modes: Through Mode (without separation), Filtering Mode (targeted analysis, resolution > 100) and Scan Mode (non-targeted analysis, resolution > 250) at a reasonable speed. Particularly, to our knowledge this new filtering mode is the first of its kind for high resolution continuous ion selection based on their cross sections.

**Methods**: UMA was designed having two parallel 2-dimensional drift channels using counter flow method which can separate ions with different mobility. Through mode was used for normal mass analysis without mobility separation, for which high electric field gradient in two channels push ions pass through UMA vertical to the gas flow direction. Scan mode was used for non-targeted mobility analysis, for which 1st channel was used for accumulating and transferring ions and 2nd channel was used for mobility analysis. Filtering mode was used for targeted mobility analysis, for which only ions with a certain mobility can pass the entire device and are selected with relatively high resolution.

**Preliminary Data**: In this presentation we show the performance of UMA in simulations. The operation modes were simulated using Fluent and SIMION combined simulation. Ansys Fluent 16 was used for gas dynamic simulation and SIMION 8.1 was used for ion trajectory simulation. In the scan mode simulation, the m/z:720 with different close collision cross section (CCS): $2.11 \times 10^{-15}$ and $2.13 \times 10^{-15} \text{m}^2$ were used and the resolution is over 200 at 40ms scan time. In filtering mode simulation, the m/z:720 with different close CCS (collision cross section): $2.09 \times 10^{-15}, 2.11 \times 10^{-15}$ and $2.13 \times 10^{-15} \text{m}^2$ were used and the resolution is about 100. In through mode simulation, the m/z of the ions used is 302, 720 and 1822, respectively. Ion transmission efficiency is near 100% for all samples. The retention time is as short as 70us for m/z:302, 120us for m/z: 720 and 220us for m/z: 1822.

**Novel Aspect**: First high-resolution mobility filter based on cross-section, using counter flow mobility approach. And fast switching capability among three operation modes.
**WP 467 Chemical kinetic and ion transport simulations: Temperature dependence of ion mobility and its impact on cluster equilibria**

**Time:** WP 467 10:30am - 2:30pm   Wed, Jun 06

**Authors:** Duygu Erdogdu¹; Walter Wisssdorf¹; Florian Stappert¹; Hendrik Kersten¹; Thorsten Benter¹; Bradley B. Schneider²; Tom Covey²

**Institutes:** ¹Bergische Universität Wuppertal, Wuppertal, Germany; ²SCIEX, Concord, ON

**Introduction:** Ion separation in differential ion mobility spectrometry (DMS) is based on the ion mobility under alternating electric field conditions. In chemically reactive systems (e.g. proton-bound water clusters), the field dependent ion mobility of individual species as well as cluster formation/ destruction rates have an impact on the observed ion mobility. Simulations were performed to address the cluster effect in detail, but the temperature dependence of the ion mobility of individual cluster species was not considered. Therefore, new ion transport simulations were performed taking into considerations both effects. Calculating the compensation-voltage (CV) in dependence of the separation-voltage (SV) allows to predict the Alpha function, which represents the field dependent ion mobility.

**Methods:** Using a newly developed code, simulations of ion transport and chemical reactions in a DMS cell were performed. To characterize the kinetics of the water cluster system, the Reaction Simulation (RS) extension to the charged particle solver SIMION was used. The new code considers the cluster effect and the influence of the field dependent effective ion temperature on the ion mobility. The simulation result analysis was executed with custom programs. To calculate the space charge interaction between particles in ion transport simulations, a custom implementation of a Barnes-Hut tree method was used. It is furthermore planned to integrate a fast multipole method into the space charge calculation, which will increase the number of simulated particles significantly.

**Preliminary Data:** The effective ion temperature is strongly affecting the cluster system equilibrium. The mean cluster size decreases at high effective ion temperature, which results in higher effective ion mobilities. In contrast, the mobility of the individual clustered species decreases with the effective ion temperature due to the well-established hard sphere behavior of individual ions. Preliminary simulations of the system of proton bound water clusters with linearly decreasing ion mobilities of the individually clustered species suggest that the hard sphere behavior of individual particles significantly counters the net effect of the chemical clustering in DMS separation stages. This is dependent on the operational conditions within the DMS stage: At elevated background gas temperature and therefore reduced mean cluster size, the simulated CV becomes positive with increasing SV. In contrast, elevated water mixing ratios yield negative simulated CVs, which imply a dominance of the chemical cluster effect. Numerical simulation results show that neither the cluster effect nor the hard sphere effect alone is sufficient to accurately model the ion transport dynamics in a DMS stage. In addition to refined mathematical models for the field dependent ion mobility of individual cluster species, experimental measurements are presented to validate and support the numerical results.

**Novel Aspect:** Numerical simulations of temperature dependent ion mobility, chemical dynamics and transport of ions through a DMS cell.

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**ThP 329 Operation and development of Ion-Mobility Orbitrap Mass Spectrometer**

**Time:** ThP 329 10:30am - 2:30pm   Thu, Jun 07

**Authors:** Jacob W. McCabe¹; Michael L. Poltash¹; Arthur Laganowsky¹; David H. Russell¹

**Institutes:** ¹Texas A&M University, College Station, TX

**Introduction:** Ion mobility mass-spectrometry (IM-MS) has developed into a multifunctional tool for the characterization and analysis of native intact protein complexes; however, current native IM-MS platforms do not possess the desired mobility and mass resolving power required for studies of macromolecule complexes encountered in structural biology. Here, we describe the development and operational parameters of a high-resolution IM-Orbitrap MS specifically designed to meet the analytical figures of merit required for the analysis of large protein complexes. Ions formed by native-ESI are analyzed using a homebuilt drift tube IM analyzer and then guided to the Orbitrap HCD cell by an octupole followed by mass analysis using standard Orbitrap acquisition modes.

**Methods:** Ion optics of the IM-orbitrap MS instrument were optimized using Simion 8.1 and machined in-house. Ions were generated using a nano-ESI source and transmitted through a heated capillary then into a RF ion funnel prior to IM DT. Initial IM experiment were carried out using a 58cm periodic-focusing ion guide drift tube (PFIG-DT). An Arduino Leonardo microcontroller is used to modulate the dual gate IMS configuration, ensuring synchronization of the IMS and orbitrap to overcome the inherent duty cycle mismatch; Orbitrap mass analysis is hundreds of milliseconds whereas IM separation is tens of milliseconds. The primary advantage of a dual gate system is the ability to directly obtain drift time measurements required for first-principle collision cross-section measurements.
Preliminary Data: This presentation describes the challenges and successes experienced during the early instrument development and establishing operational parameters required for coupling DT IM to an Orbitrap MS that will make possible both high resolution IM and MS. Results for a variety of systems ranging from peptides to protein complexes will be discussed and will illustrate the efficacy of the ion source coupled directly to the HCD Cell. Coupling IMS directly to the HCD cell of the instrument maintains the original instrument operation and performance during the entirety of the instrument's development. Evaluation of the new interface showed retention of mass performance and native like charge states. Using IM-TOFMS, the IM separated ion are mass analyzed as they are eluted from the DT, i.e., IM separation is slow, tens of milliseconds, whereas TOF mass analysis is very fast, 10-100 microseconds. The duty-cycle mismatch for IM-orbitrap can be overcome by using a dual gate strategy. Gate 1 pulses a packet of ions into the DT for IMS separation and Gate 2 is used to allow mobility selected ion packets into the HCD cell for mass analysis. The delay time between pulsing of Gate 1 and Gate 2 represents the drift time of mass-analyzed ions and is modulated per mass scan sample the entire drift time of interest. Accumulation of multiple packets of ions in the HCD cell extents the lifetime of ions sampled in the MS; however, the conformation(s) of the trapped ions is defined by the IMS arrival time distributions, and any changes in conformation in the HCD cell are irrelevant.

Novel Aspect: This IM-orbitrap provides access to high-resolution IM-MS measurements of intact protein complexes while utilizing a first-of-its-kind interface to an Orbitrap.

ThP 462 Experimental Observation of the Effects of Translational and Rotational Electrode Misalignment on a Planar Linear Ion Trap Mass Spectrometer
Time: ThP 462 10:30am - 2:30pm Thu, Jun 07
Authors: Yuan Tian1; Joshua S McClellan1; Trevor K Decker1; Qinghao Wu1; Abraham L De la Cruz Hernandez1; Aaron R Hawkins1; Daniel E Austin1
Institutes: 1Brigham Young University, Provo, UT

Introduction: Miniaturization of ion traps (IT) poses several obstacles to achieving optimum IT performance. At such reduced size scales, electrode misalignment can easily affect ion trap capacity, sensitivity and electric field accuracy. The Two-Plate Linear Ion Trap (LIT) is an ideal candidate to study the effects of electrode misalignment at the miniature scale because of the simplicity of alignment, having only 6 degrees of freedom (three rotational and three translational) between the two patterned plates.

Methods: Glass plates were lithographically patterned with aluminum lines as electrodes. High precision motorized actuators were used to test electrode misalignment on five of the six degrees of freedom. Samples tested includes a mixture of toluene and deuterated (D8) toluene a and a mixture of xylenes. One plate was fixed while the other plate was adjusted along each of the different degrees of freedom. The five degrees of freedom were labeled: x, y, z, pitch and yaw. Experimental results were compared to previously reported simulations using SIMION.

Preliminary Data: The different degrees of freedom presented different contributions to the trapping performance. Pitch had the greatest impact on mass resolution and intensity at different pitch angles. Small deviations were found with x-displacement as well as with z-displacement; however, x-displacement had the greatest effect on ion ejection. Y-displacement had the greatest contribution on the ion detection efficiency. Finally, yaw had an effect degrading mass resolution.

Novel Aspect: First experimental results on the effects of electrode misalignment with multiple degrees of freedom in two-plate linear ion trap.

ThP 480 Development of a portable MALDI-TOF-MS for microbial identification
Time: ThP 480 10:30am - 2:30pm Thu, Jun 07
Ko-Keng Chang* [1] [2]; Yi-Hong Cai [1]; Cheng-Chih Hsu [2]; Yi-Sheng Wang [1]
[1] Genomics Research Center, Academia Sinica, Taiwan; [2] Chemistry Department, National Taiwan University, Taiwan
Authors: Ko-Keng Chang1,2; Yi-Hong Cai1; Cheng-Chih Hsu2; Yi-Sheng Wang1
Institutes: 1Genomics Research Center, Academia Sinica, Taiwan; 2Chemistry Department, National Taiwan University, Taiwan

Introduction: MS-based microbial identification became more useful because of its low price and high speed. It is most done by Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS). But due to MALDI-TOF-MS instrument's size and price, this method has its limitation. We developed a portable MALDI linear TOF-MS instrument for microbial identification or other applications. The maximum length of this instrument is 50 cm and weight approximately 10 kg. Also the cost will be significantly lower than commercial instrument, making easier to popularize.

Methods: This portable MALDI-TOF-MS instrument was self-designed. Performance was estimated by comprehensive calculation. The vacuum system is an 80L/s turbomolecular pump with two diaphragm pumps for rough pumping. Ions are
produced by MALDI ion source, this MALDI ion source is equipped with a compact pulsed DPSS laser and X-Y moving mechanism. Drift through a 40 cm long flight tube, arrive at the detector. The detector of this instrument is the bipolar ion detector (BID), which is able to work under low vacuum condition and has previously been demonstrated to be more sensitive than microchannel plate detector.[1]

Preliminary Data: The design of instrument was done by 3D CAD system. Simulation of electrical field and charged particle trajectories was done and optimized by SIMION. Parts are self-made or manufactured by local factories. Microbial identification have been tested by commercial instrument which proves its accuracy and speed. For microbial identification, the required mass range is 2 thousand to 20 thousand Dalton, and does not require high resolving power (2,000 is sufficient). By two-ion case calculation, we estimate the optimum ion acceleration voltage is 12 to 15 kV for sufficient resolving power and detection efficiency. High voltage power supply with pulse voltage function was developed for ion acceleration. Vacuum chamber was made by aluminum alloy to reduce weight. The compact and low-power vacuum system is tested, it can generate high vacuum which the ion mean free path is enough for drifting. Overall testing of the instrument is in progress.[1] Ming-Hsin Li et al., Bipolar Ion Detector Based on Sequential Conversion Reactions, Anal. Chem., 79(4) 2007, 1277-1282

Novel Aspect: The portable MALDI-TOF-MS is compact and low price, allowing wider variety of applications.

ThP 481 The fine-structure ion carpets for the transport of ions at atmospheric pressures
Time: ThP 481 10:30am - 2:30pm Thu, Jun 07
Authors: Sergey Poteshin1; Anna Burykina2
Institutes: 1National Research Nuclear University MEPHI, Moscow, Russian Federation; 2National Research Nuclear University MEPHI, Moscow, Russia

Introduction: The vast majority of ion losses take place in the range close to atmospheric pressure on a way from API to analyzer. Also this problem is one of main limiting factor of the sensitivity for the ion mobility spectrometry/mass spectrometry. Thus development of an ion guide operating and with mainly use of of RF fields is especially attractive. Such systems can be used not only for transportation, but also for storing or accumulating ions. The main problem in developing ones is a need to apply the high frequencies and amplitudes of the supply voltages. Here we consider a focusing system based on the flat fine-structure electrode ion carpet with acceptable dissipation of reactive power below 50 W/cm².

Methods: Estimation The efficiency of the electrodes was evaluated by calculating the pseudopotential, which should create an electrode to hold the ion cloud with a specified space charge. Buffer gas and damping of the motion were taken into account for pseudopotential model. We use the equations suggested by group of R.D. Smith in [doi:10.1002/mas.20232] for maximal pseudopotential value above the electrode surface. Simulation The ion trajectories in the gas filled area in RF electric field were simulated using SIMION 8.1 with own modified HS1 Collision Model code based on Monte-Carlo calculation method. Modification of the standard HS1 program allowed one to significantly accelerate the calculation of trajectories at the atmospheric pressure without loss of accuracy.

Preliminary Data: Numerical simulations and estimations allowed us to estimate a value of damping pseudopotential needed to transport the ions with m/z>200 over the surface of a fine structure ion carpet. This value was shown to be achieved by a fine structure ion carpet with 20 µm distance between centers of adjacent electrodes. Released reactive power is about 50 W/cm² for m/z≈200 and still within the limits permissible for convective heat dissipation. Modified SIMION 8 HS1 code allowed us to simulate ion transport in RF field basing on Monte-Carlo method calculation of hard-sphere collision at atmospheric pressure without significant time consumption. SDS model gave the result with unacceptable errors in condition of high frequency strong RF electric fields. As a result of numerical simulation RF, voltage parameters (Vn, f) were found for effective transport of ions with different masses and collision cross sections over a surface of a fine structure ion carpet. Theoretical value of damped effective pseudopotential is in good agreement with the data obtained from the results of a numerical simulation. A fine structure ion carpet is expected to be constructed by direct writing lithography and vacuum metal deposition followed by resist liftoff for future experimental study.

Novel Aspect: Focusing system of ions at atmospheric pressures based on the fine-structure electrode with track pinch 10 µm

ThP 513 Charge detection mass spectrometry of microparticles using printed circuit board electrode arrays
Time: ThP 513 10:30am - 2:30pm Thu, Jun 07
Authors: Elaura L. Gustafson1; Halle V. Murray1; Daniel E. Austin1
Institutes: 1Brigham Young University, Provo, UT

Introduction: Charge-detection mass spectrometry (CD-MS) can be used to determine the charge and mass of microparticles. One strategy to determine mass includes the use of a DC potential region between sensing electrodes to
accumulate quadrupole. A Mass of particle sizes and charges, the can be increased in a FT frequency enhancement of 86% however experimental data using cesium iodide clusters will be used to compare true experimental mass ranges.

the decreased trap length. Simulations of experiments, mirror simulations are heavily influenced by the length of the trap and the technique used to trap ions in the mass analyzer. In these range in FT spectra with the 5" and 2.5" ELIT were used to determine relative frequency enhancements.

has been demonstrated using tetraoctylammonium (TOA), bradykinin, and insulin. Direct comparison of TOA, Bradykinin, miniaturized ELIT was developed that is half the length (2.5") of the previous trap (5"). A filter was used to remove microparticles, a beam tube to establish correct pressure and flow, and the CD-MS instrument in a vacuum chamber. This charge detector will provide the charge, velocity and kinetic energy of the particles. The mass of the particles can then be derived and calculated from the kinetic energy and charge. Instrument performance has been simulated using SIMION ion trajectory software. A multi-axis micropositioner is used to observe effects of particle position on the measurement, including off-angle scatter and lensing effects.

Preliminary Data: Instrument performance is simulated using SIMION ion trajectory software. Parameters such as initial kinetic energy, gas flow, drag and particle density were adjusted to match expected Martian conditions. For a given acceleration voltage, particles with m/z too high are not accelerated or decelerated enough for the resulting signal delay to be discernible (less than 5-10% change in velocity). The charge can still be measured, but only a lower-limit to the particle’s mass determined. Particles with m/z too low are deflected onto the circuit board and bounce before returning to the gas flow. These will produce an erratic signal and are not usable for analysis. Between these extremes is a range of m/z values suitable for producing analyzable signals. In order to monitor a wide range of particle sizes and charges, the DC voltage in the acceleration/deceleration region is adjustable over the range 0.1 to 360 V. Though this is working very close to the minimum in the Paschen curve for Mars atmospheric conditions, 360 V is sufficient to produce measurable deceleration/acceleration of particles up to 11 μm in diameter with at least 10,000 charges.

Novel Aspect: First evaluation of printed circuit board based charge detection for measuring the mass of individual microparticles.

ThP 519 Enhanced Resolution via Miniaturization of a Fourier Transform Electrostatic Linear Ion Trap Mass Spectrometer

Time: ThP 519 10:30am - 2:30pm Thu, Jun 07
Authors: Joshua T. Johnson¹; Kenneth W. Lee¹; Jay S. Bhanot¹; Scott A McLuckey¹
Institutes: ¹Purdue University, West Lafayette, IN

Introduction: In a Fourier transform electrostatic linear ion trap (FT-ELIT), ions oscillate between two opposing reflectrons. The frequency at which the image charge is induced on a centrally located detector is related to ion mass-to-charge. Resolution in FTMS is dependent on transient acquisition time as well as ion frequency. In a FT-ELIT, the axial length of the mass analyzer directly influences the frequency of trapped ions. For ions injected at approximately the same kinetic energy, reduction of the axial dimensions of the mass analyzer increases ion frequencies and results in a concomitant enhancement in resolution per unit time. In the new miniaturized FT-ELIT, the length of the previous trap was halved resulting in frequency and resolution enhancements of 86%.

Methods: All experiments were carried out on a home-built Fourier transform electrostatic linear ion trap. Ions were generated via nanoelectrospray ionization and collisionally cooled with nitrogen gas in an accumulation quadrupole. A bunched ion packet was injected into the ELIT where the image charge was digitized and Fourier transformed to yield a mass spectrum. Frequency enhancements were demonstrated by comparing data collected on two separate ELIT mass analyzers, one with an axial length of 5” and a miniaturized ELIT with an axial length 2.5”. Mass ranges for both trap geometries were simulated using SIMION v8.1. Resulting transients were analyzed and processed using FTDataPro (Sciex, Concord, ON) and compared to determine the relative frequency and resolution enhancements.

Preliminary Data: In FTMS, resolution per unit time is affected by the measured ion frequencies. Increasing ion frequencies results in higher resolution per unit time. Ion frequencies can be increased in a FT-ELIT by simply reducing the axial dimensions of the trap while keeping constant the kinetic energy in which ions are injected. Thus, a new miniaturized ELIT was developed that is half the length (2.5”) of the previous trap (5”). A frequency enhancement of 86% has been demonstrated using tetraoctylammonium (TOA), bradykinin, and insulin. Direct comparison of TOA, Bradykinin, and insulin frequency spectra with the 5” and 2.5” ELIT were used to determine relative frequency enhancements. Mass range in FT-ELIT experiments is dictated by the time-of-flight acceptance range of the trap. This acceptance range is heavily influenced by the length of the trap and the technique used to trap ions in the mass analyzer. In these experiments, mirror switching was used and therefore the TOF acceptance region is the entire axial length of the ELIT device. Thus, the mass range in the new Mini-ELIT is expected to decrease at any given mirror switching time because of the decreased trap length. Simulations (SIMION v8.1) indicate an overall mass range decrease of approximately 30%, however experimental data using cesium iodide clusters will be used to compare true experimental mass ranges.
**Novel Aspect:** Resolution enhancement in a Fourier transform electrostatic linear ion trap with reduced axial dimensions

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**ThP 521 Simulation of collisional interactions of background gas mixtures with trapped ions**

**Time:** ThP 521 10:30am - 2:30pm  Thu, Jun 07

**Simulation of collisional interactions of background gas mixtures with trapped ions**

**Authors:** Thorsten Benter; Walter Wissdorf; Marco Thinius; Hendrik Kersten

**Institutes:** ¹Bergische Universität Wuppertal, Wuppertal, Germany

**Introduction:** Ion traps are among the most common mass analyzers in commercial mass spectrometric instruments. Buffer gas with low molecular weight is often used in such instruments to collisionally cool analyte ions during the trapping process. In contrast, collisions with heavier background gas particles can lead to unwanted collisional excitation and even ejection of ions from the trap. In commercial setups with in-trap ionization, the presence of complex gas mixtures in the trap is inevitable. Experimental observations of basic heating effects are described in the literature, but so far there is no systematic investigation of the collisional effects of gas mixtures in ion-traps. We present numerical simulations to systematically investigate these effects.

**Methods:** Motion of analyte ions in a commercial quadrupole ion trap with neutral gas mixtures present are simulated with SIMION. Further, simulations with an idealized quadrupolar trapping field are performed in a custom simulation framework with a Verlet-type trajectory integrator. In both cases, the interaction between background gas and ions are modeled with a hard sphere collision model adapted for variable mixtures of background gases. The simulations and the result analysis are automated to allow systematic variations of simulation parameters, e.g., configuration of the trap field voltage, frequency or the mass ratio between ions and the background gas components.

**Preliminary Data:** The modified versions of the collision models were qualified with verification simulations. First productive simulations of the ion trap with analyte ions of m/z = 40 and different admixtures of neutral Helium (M = 4 Da) and the neutral analyte gas (M = 40 Da) demonstrated collisional cooling and heating effects in dependence of the partial pressures of the neutral gas components. Effects as for example ion motion decorrelation, changes in the averaged ion oscillation radius, and ion ejection from the trap were observed in the simulations. First results suggest, that most of the effects caused by the presence of the background gas components scale linearly with the respective partial pressures of the individual gases. Consequently, an in-trap ionization technique can probably tolerate comparably high concentrations of heavy analyte- and contaminant-species in the trap without severely affecting the mass analyzer performance. Systematic simulations allow to investigate the dependence of quadrupole ion trap analyzer performance as well the extent of unwanted ion ejection from the trap in dependence of the background gas composition. Furthermore, the developed simulation frameworks allow to systematically investigate other ion trap devices, particularly linear ion traps, and elements of ion transfer stages, e.g., ion funnels or multipole devices.

**Novel Aspect:** Systematic investigations of the impact of the background gas composition on the ion dynamics in quadrupole ion traps.

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**ThP 523 Fundamentals of Cyclotron-Frequency FT-ICR MS**

**Time:** ThP 523 10:30am - 2:30pm  Thu, Jun 07

**Authors:** Konstantin O. Nagornov; Anton N. Kozhinov; Edith Nicol; Yury O. Tsybin

**Institutes:** ¹Spectroswiss, Lausanne, Switzerland; ²Ecole Polytechnique, Palaiseau, France

**Introduction:** Development of space-charge tolerant FTMS technologies is indispensable for next-generation MS applications and further progress of FTMS. Recently, we introduced FT-ICR MS at the cyclotron frequency instead of the reduced cyclotron frequency, using the narrow-aperture detection electrodes (NADEL) ICR cells. SIMION and PIC simulations demonstrated that ion spatial re-distribution during ion detection in highly non-quadratic trapping potentials inside the NADEL ICR cells forms novel types of dynamic ion structures – elliptic cylinders and ion slabs. Experimental studies on the two FT-ICR MS instruments demonstrated high frequency stability and ion motion coherence achievable during the long detection periods. Here, we describe further in-silico characterization of FT-ICR MS at the cyclotron frequency, including NADEL ICR cell geometries with multiple narrow-aperture detection electrodes.

**Methods:** SIMION simulations were conducted for NADEL ICR cells equipped with three, four, eight, and sixteen narrow-aperture detection electrodes. A multi-dipolar, tripolar, quadrupolar, quadrature, and octupolar ion detection and excitation schemes, in conjunction with a DC sidekick for excitation of ion magnetron motion, were employed. Motion of 100-1000 ions with up to 50% spread in their initial velocities was simulated for up to 10 kV trapping voltages. For comparison, we simulated ion motion and detection also in the conventional and dynamically harmonized cylindrical ICR cells. Inhomogeneous magnetic field with a quadratic dependence along the cell axis was simulated using a model of the Helmholtz coil. Ion trajectories visualization, processing of time-domain signals, and data analysis were performed using in-house developed software.
**ThP 526 Nonlinear Ion Trap Stability Diagram Mapping by Trajectory Harmonic Content**

**Time:** ThP 526 10:30am - 2:30pm Thu, Jun 07

**Authors:** Robert H Jackson¹; Stephen A Lammert²

**Institutes:** ¹Instrumental Design Physics, LLC, Littleton, MA; ²PerkinElmer Inc., American Fork, UT

**Introduction:** Stability diagrams are convenient constructs to study the effects of non-linear contributions to ion trapping fields. These fields show up as valleys/chasms that permeate the stability region or as stability boundary shifts. These artifacts are amplified with increasing non-linear character and can be employed as an observable metric in attempts to control, design or minimize the amount of non-linear character in a given device. Typically, this is achieved by simulating an ion’s full path from the cooled center to ejection or by determining whether an ion survives a prescribed time. This new approach uses harmonic content to predict the position of the stability boundary, dependent on its initial conditions, and without requiring the ion to become unstable.

**Methods:** Ion traps are modeled in SIMION® 8.1 (8.2 extensions), employing harmonic inversion (HARMINV, S.G. Johnson, MIT) of single ion trajectories at each operating point (Vrf, Vdc). The \( \beta_z = 0 \) and \( \beta_r = 0 \) boundaries are determined by observing the harmonics of the ion trajectory motion stepping Vdc along constant rf voltage lines. Using these frequency versus Vdc curves we can project to the appropriate \( \beta_z = 0 \) or \( \beta_r = 0 \) point at the boundary of the stability diagram. Similarly, we determine the \( \beta_z = 1 \) or \( \beta_r = 1 \) boundaries stepping the rf voltage at constant dc. These harmonic maps made at several initial conditions show how the effects of nonlinear fields grow as the ions are started further from the trapping center.

**Preliminary Data:** We have measured both RF and DC scan lines using mass 99da in a simulation of the toroidal ion trap starting the ions at the trapping center with a 0.01 eV kinetic energy in the z direction. Two dc scans are made at an Vrf = 60Vp, one stepped from Vdc = 0 to 7.25V in 0.25V steps and the other Vdc = 0 to -7.25V. Each of the dc scans show parabolic like curves of dc voltage versus harmonic frequency centered around 0, 2, and 4 MHz with the \( \beta_z = 0 \) and \( \beta_r = 0 \) conditions determined by inspection to be +/-5.4Vdc. Similarly, there are three RF scan lines made with Vdc = 0, +2, and -2 volts, \( \beta_z = 1 \) and \( \beta_r = 1 \) conditions determined by parabolic like curves of Vrf versus harmonic frequency centered around -1, +1, and +3MHz \( \beta_z = 1 \) or \( \beta_r = 1 \) conditions at Vrf = 149Vp for Vdc= 0V, Vrf= 150Vp for the Vdc=-2V, and Vrf = 146Vp for Vdc= -2Vdc. These measurements can also be made such that the separate r and z motion harmonics are identified. The stability boundaries here were estimated by visual inspection, however for detailed scans of the entire stability region we are developing a mathematical method for identifying and fitting these parabolic like curves, which would not only estimate the stability boundaries, but provide the \( \beta_z \) and \( \beta_r \) values throughout the stability diagram from which we can derive the Mathieu parameters \( a_z \), \( q_z \), \( a_z \), and \( q_z \).

**Novel Aspect:** Mapping of separate r and z harmonic content over the stability region with initial condition dependence.