

Report of activities carried out at the Georgia Institute of Technology as a part of grant # NSF-CHE- 0410427, Subcontract with Stanford University (G-33-C52).

Final report

To: Prof. Richard N. Zare, Stanford University.

From: Prof. Facundo M. Fernandez, Georgia Institute of Technology.

Research Activities

A summary of accomplishments during the development of this project is as follows:

1. We have successfully built and characterized the first resistive glass standalone ion mobility spectrometer using Faraday plate detection, and characterized its ion density distribution, effect of experimental variables on performance, and resolving power. Resolving power per unit length is one of the highest ever reported in the literature with an instrument of this type.
2. We have developed a unique multiplexing/demultiplexing scheme based on arbitrary modulation waveforms and pseudoinverse deconvolution. The main advantage of this approach is the ability of changing the duty cycle arbitrarily and thus improving signal to noise ratios by up to 10x in comparison with the conventional, non-multiplexed, experiment.
3. We have identified the factors contributing to non-ideal behavior in drift tube IMS for the particular instrument constructed in our lab using theoretical considerations based on ion diffusion and ion gating processes.
4. Our results have been published in top-rated peer reviewed journals (3 publications), and a book chapter which provides a tutorial on IMS multiplexing.

Synergistic Activities:

Member and Chair Elect (2008) of the organizing committee for the Asilomar Conference on Mass Spectrometry (2008-2011).

Member of the Editorial Advisory Board of *The Analyst*, Royal Society of Chemistry (2008-2012).

Member of the 2010 ACS Franklin H. Field and Joe L. Franklin Award Committee for Outstanding Achievement in Mass Spectrometry (2010-2011).

Member of the 2008 Program Review Committee for the 56th ASMS Conference on Mass Spectrometry and Allied Topics.

Chair of the "Complex Systems" session at the 20th ASMS Sanibel Conference on Mass Spectrometry: Ion Mobility and Related Emerging Areas, January 18–21, 2008, Daytona Beach, FL.

Chairs of the "Developments in Ion Mobility: Instrumentation and Theory" session at the 56th ASMS Conference on Mass Spectrometry and Allied Topics, Denver, CO, June 1-5, 2008.

Member of the 2007 Harsh Environment Mass Spectrometry Workshop Organizing Committee.

Participants

Facundo M. Fernandez (coPI)

Mark Kwasnik (Graduate student). Graduated successfully in May 2010. Now employed at Solvay Group.

Joseph Caramore (REU undergraduate), now in graduate School.

Publications

- “Performance, Resolving Power and Radial Ion Distributions of a Prototype Nanoelectrospray Ionization Resistive Glass Atmospheric Pressure Ion Mobility Spectrometer” Mark Kwasnik, Marc Gonin, Katrin Fuhrer, Kathy Barbeau, Facundo M. Fernández, *Anal. Chem.*, **2007**, 79, 7782-7791.
- “Digitally-Multiplexed Nanoelectrospray Ionization Atmospheric Pressure Drift Tube Ion Mobility Spectrometry”, Mark Kwasnik, Joe Caramore, Facundo M. Fernández*, *Anal. Chem.* **2009**, 81, 1587-1594.
- “Multiplexed Ion Mobility Spectrometry and Ion Mobility Mass Spectrometry”, Mark Kwasnik, Glenn, A. Harris, Facundo M. Fernandez. *Accepted* for “Ion Mobility-Mass Spectrometry. Theory and Applications” by Charles L. Wilkins and Sarah Trimpin.
- “Theoretical and Experimental Study of the Achievable Separation Power in Resistive-Glass Atmospheric Pressure Ion Mobility Spectrometry”, Mark Kwasnik, Facundo M Fernández, *Rap. Comm. Mass. Spectrom*, **2010**, 24, 1911-1918.

Presentations at Meetings and Symposia

1. Characterization of the Resolving Power and Resolution of a Monolithic Resistive Glass Drift Tube Ion Mobility Spectrometer”, Mark Kwasnik and Facundo M. Fernández, 58th ASMS Conference on Mass Spectrometry and Allied Topics; May 23-27, 2010; Salt Lake City, UT.
2. “Enabling Tools for Proteomics and Metabolomics”, Facundo M. Fernández, *REMTEC 2009, Remediation Technology Summit*, Mar. 3-5, 2009; Atlanta, GA.
3. “A Variable Duty Cycle Digital Multiplexing Method for Atmospheric Pressure Drift Tube Ion Mobility Spectrometry” Mark Kwasnik, Joe Caramore, Facundo M. Fernandez, *SERMACS 2008*, Nov. 12-15, 2008, Nashville, TN.
4. “Investigation of Alternate-Construction and Variable Duty Cycle Gating Waveforms for Digitally-Multiplexed Atmospheric Pressure Drift Tube Ion Mobility Spectrometry”, Mark Kwasnik, Facundo M. Fernández, *2008 Conference of the Federation of Analytical Chemistry and Spectroscopy Societies*; Sept. 28-Oct. 2, 2008; Reno, NV.
5. “Signal to Noise Ratio Gains in Digitally-Multiplexed Atmospheric Pressure Drift Tube Ion Mobility Spectrometry”, Mark Kwasnik, Facundo M. Fernández, Joe Caramore, *56th ASMS Conference on Mass Spectrometry and Allied Topics*; June 1-5, 2008; Denver, CO.
6. “Digital Atmospheric Pressure Resistive Glass Ion Mobility Spectrometry: Instrumentation, Multiplexing and Data Deconvolution”, Mark Kwasnik, Facundo M. Fernandez, *20th ASMS Sanibel Conference on Mass*

- Spectrometry: Ion Mobility and Related Emerging Areas, January 18–21, 2008, Daytona Beach, FL.
7. "Tecnologías Emergentes para Análisis Ambiental, Proteomics y otros "Omics": Espectrometría de Masas por Ionización Directa, Electroforesis Capilar Multiplexada y Electroforesis en Fase Gaseosa.", Fernández, F. M., Nyadong, L. N., Pierce, C., Kwasnik, M., Hampton, C. Y., Navare, A., Zhou, M., II Congreso Iberoamericano y IV Congreso Argentino de Química Analítica, Aug. 27-30, 2007, Buenos Aires, Argentina.
 8. "Frontiers in Mass Spectrometry: Direct Ionization, Quantitation, and Multidimensional Separations", Facundo M. Fernández, Christina Hampton, Leonard Nyadong, Carrie Pierce, Mark Kwasnik, Arti Navare, Coca Cola-Chemistry Forum, May 8, 2007.
 9. "A Novel Resistive Glass Atmospheric Pressure Ion Mobility Spectrometer", Mark Kwasnik, Joe Caramore Katrin Fuhrer, Marc Gonin, Katherine Barbeau, Facundo M. Fernandez, 6th Harsh-Environment Mass Spectrometry Workshop, September 17-20, 2007, Cocoa Beach, Florida.
 10. "Resistive Glass Atmospheric Pressure Ion Mobility Spectrometry of Iron-Siderophore Complexes", Mark Kwasnik, Ignacio Zuleta, Katrin Fuhrer, Marc Gonin, Katherine Barbeau, Richard N. Zare, Facundo M. Fernández, *Gordon Research Conference. Biomolecules in the Gas Phase. Mass Spectrometry, High Resolution Spectroscopy and Theory*, Bates College, Lewiston, ME, July 22-27, 2007.
 11. Characterization of a Prototype Resistive Glass Atmospheric Pressure Ion Mobility Spectrometer with Corona Discharge and Nanoelectrospray Ion Sources", Mark Kwasnik, Katrin Fuhrer, Marc Gonin, Facundo M. Fernandez, *2007 ASMS Conference*, June 3-7, 2007, Indianapolis, IN.

Outreach activities:

1. "Machines that Make Invisible Molecules Visible", Facundo Fernandez (Keynote Speaker), *42nd Annual Southeast Regional American Chemical Society 2010 Undergraduate Research Conference*, April 8-9, Kennesaw State University, Kennesaw, Georgia.
2. In 2005 we hosted a high School teacher through the GIFT program at GT
3. The coPI has visited groups of Hispanic students at high schools to discuss career paths.
4. Recruited a bright REU student from Muhlenberg College, who is now in graduate school.

