

Kurt Frey

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EDUCATION

Massachusetts Institute of Technology

Cambridge, MA

PhD Chemical Engineering, February 2010

September 2005 - January 2010

MS Chemical Engineering Practice, September 2005

September 2004 - September 2005

- Graduate thesis: "Improving Thermodynamic Property Estimation through Volume Translation."
 - Eliminated numerical inconsistencies that led to prediction of aphysical properties.
 - Introduced new formulation of translation function allowing for greater flexibility in modeling.
- Economics minor: Microeconomic theory and natural resource economics.
- Awarded "Outstanding Graduate TA" academic year 2006-2007; Chemical Engineering Dept.

Ohio State University

Columbus, OH

BS Chemical Engineering, June 2004

September 1999 - June 2004

- Undergraduate thesis: "Exchange and Correlation Functional Selection in Computational Chemistry of Actinide Containing Compounds."
 - Benchmarked basis set accuracy for relativistic core small molecules containing actinides.
 - Evaluated implementation of density functional algorithms in Gaussian for actinide systems.
- Computer science minor: Software and algorithms.
- Recipient of senior and sophomore "Award for Academic Excellence"; Chemical Engineering Dept.
- Selected as sophomore "Outstanding Mathematics Student"; Mathematics Dept.

EXPERIENCE

Argonne National Laboratory

Argonne, IL

Postdoctoral Appointee

February 2010 - January 2013

- Implemented mixed potential model for degradation and dissolution of spent fuel waste forms.
- Created systems analysis application for analyzing nuclear fuel reprocessing facilities.
- Reformulated process simulation model for nuclear fuel reprocessing to include time dependency.
- Developed polarizable force field for molecular dynamics simulation of complex extractants.
- Analyzed production rates of chemical agent precursors using non-export controlled materials.

BP

Sunbury, United Kingdom

Contractor

May 2008 - June 2008

- Analyzed current property estimation accuracy for Exploration and Production Technology.
- Implemented property package developed during doctoral research at MIT to improve performance.

Schlumberger

Cambridge, MA

Research Scientist

June 2006 - December 2006

- Created model to simulate the advection-diffusion of fluid flow through realistic porous networks.
- Applied model to novel three-dimensional lattice representation of Berea sandstone.
- Predicted phenomena observed in NMR flow propagator analysis of sandstone.

Novartis

Basel, Switzerland

Student Intern

July 2005 - September 2005

- Created model with interface for pilot plant capacity and efficiency; predicted future bottlenecks.
- Analyzed current implementation of process analytic technology for use in powder pharmaceuticals.
- Formulated novel dry powder mixtures for testing inhalation performance, in-line quality assurance.

Cabot Corporation

Student Intern

Billerica, MA

May 2005 - June 2005

- Explained and eliminated undesired phenomena observed during analysis of ink formulations.
- Characterized abilities of novel device to evaluate poly-dispersed colloidal systems.

Ohio State University

Co-curricular Project Aide

Columbus, OH

January 2000 - December 2002

- Coordinated and implemented special projects for Honors & Scholars center.
- Managed applications and interviews for Battelle/Joyce, Maximus scholarship competitions
- Evaluated applications for Honors program admission; administered database for graduation honors.

PUBLICATIONS / PRESENTATIONS

Refereed Papers

- K Frey, J Tester, "Quantitative Representation of Gibbs' Fundamental Surface for Water," *Chem. Eng. Edu.*, **2013**, in preparation.
- K Frey, J Krebs, C Pereira, "Time Dependent Implementation of Argonne's Models for Universal Solvent Extraction," *Ind. Eng. Chem. Res.*, **2012**, 51, 13219-13226.
- K Frey, J Tester, M Modell, "Density-and-temperature-dependent volume translation for the SRK EOS: 2. Mixtures," *Fluid Phase Equilib.*, **2012**, submitted.
- K Frey, J Tester, M Modell, "Density-and-temperature-dependent volume translation for the SRK EOS: 1. Pure fluids," *Fluid Phase Equilib.*, **2009**, 279, 56-63.
- K Frey, et al., "Volume translation in equations of state as a means of accurate property estimation," *Fluid Phase Equilib.*, **2007**, 260, 316-325.
- G Picard, K Frey, "Method for modeling transport of particles in realistic porous networks: Application to the computation of NMR flow propagators," *Phys. Rev. E.*, **2007**, 75, 066311.

Talks and Presentations

- "Multi-domain mixed potential model for spent fuel dissolution," AIChE Annual Meeting, Minneapolis, MN; October 2012.
- "Gibbs ensemble Monte Carlo examination of the water/n-dodecane/tributyl phosphate system," ACS National Meeting & Exposition, San Diego, CA; March 2011.
- "Time dependent implementation of Argonne's Model for Universal Solvent Extraction," AIChE Annual Meeting, Minneapolis, MN; October 2011.
- "Time dependent implementation of Argonne's Model for Universal Solvent Extraction," Argonne Postdoctoral Research Symposium, Argonne, IL; September 2011.
- "Polarizable force field development and application for simulations of interest to solvent extraction," ACS National Meeting & Exposition, Anaheim, CA; March 2011.
- "Multiparameter equation of state basis set selection," AIChE Annual Meeting, Salt Lake City, UT; November 2010.
- "Development of a polarizable force field for tributyl phosphate," Argonne Postdoctoral Research Symposium, Argonne, IL; September 2010.
- "Volume translated equation of state for supercritical fluid mixture densities," ACS National Meeting & Exposition, San Francisco, CA; March 2010.
- "Method of volume translation," ACS Green Chemistry Summer School, Golden, CO; July 2008.
- "Opportunities in energy efficiency from process simulation," MIT Energy Showcase, Cambridge, MA; April 2008.
- "Improved thermodynamic property estimation through the application of volume translation," BP Projects Academy Showcase, Cambridge, MA; October 2007.
- "Accuracy in thermophysical property estimation," National Renewable Energy Laboratory, Golden, CO; January 2006.

ACTIVITIES

Professional Development

- 4th Annual Short Course on Parallel Programming; ParLab UC Berkeley; Berkeley, CA; August 2012.
- Optimization Modeling and Integrated Process Operations; CAPD CMU; Pittsburgh, PA; May 2012.
- Postdoc-to-Faculty Workshop; ACS Education Division; Boston, MA; August 2010.
- Advanced Course on Molecular Simulation of Complex Chemical Systems; DTU CERE; Lyngby, Denmark; July 2010.
- Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects; DTU CERE; Lyngby, Denmark; January 2009.
- Green Chemistry and Sustainable Energy Summer School; ACS Green Chemistry Institute; Golden, CO; July 2008.

Service

- Skyway Conference STEM Contest Judge; Illinois Skyway Conference; Palos Hills, IL; April 2011.
- Middle School Regional Science Bowl Judge; US Department of Energy; Argonne, IL; February 2012, February 2011.
- Middle School Regional Science Fair Judge; Chicago Public Schools; Chicago, IL; January 2012.
- Hispanic Educational Outreach Volunteer; Argonne National Laboratory; Argonne, IL; October 2011, October 2010.
- SERCh Poster Competition Judge; US Department of Energy; Argonne, IL; November 2010.
- AAAS Congressional Visits Day; MIT Science Policy Initiative; Washington, DC; March 2008.
- State Science Day Judge; Ohio Academy of Science; Columbus, OH; May 2004, May 2003.
- Wonders of Our World Volunteer; Ohio State Chemistry Department; Columbus, OH; Spring 2003.

Personal Interest

- Instrumentalist (Tenor Trombone; Bass Trombone; Euphonium): Cambridge Symphony Orchestra, MIT Musical Theater Guild, MIT-Gilbert and Sullivan Players, MIT Concert Band, Somerville Brass Quintet, Summer Street Brass Quintet, OSU University Band, OSU Athletic Band, OSU Marching Band.
- Community volunteer: Lakeview Pantry, National Braille Press, Perkins School for the Blind, Columbus Recreation and Parks Department.
- Voice talent (Narrow IPA; Standard American; Proper American): Narrations, Voice-over, ADR.
- Club Sports (Ice hockey; Football; Basketball; Softball; Volleyball; Bowling): Argonne Club, MIT Intramural Athletics, Ohio State Intramural Athletics