

Donald P. Visco, Jr.

Education

Ph.D., June 1999

Department of Chemical Engineering

State University of New York at Buffalo, Buffalo NY

Thesis Advisor: Dr. David A. Kofke

Thesis Title: *Thermodynamic and Molecular Modeling of Hydrogen Fluoride*

B.S., May 1992 (*cum laude*)

Department of Chemical Engineering

State University of New York at Buffalo, Buffalo NY

Professional Experience

University of Akron

Professor of Chemical and Biomolecular Engineering, January 2011—Present

Dean, College of Engineering, July 2017 – August 2018

Interim Dean, College of Engineering, July 2016 – July 2017

Associate Dean of Undergraduate Studies, College of Engineering, January 2011 – July 2016
Akron, OH

Tennessee Technological University

Interim Associate Dean, College of Engineering, May 2010 – December 2010

Professor of Chemical Engineering, June 2008 – December 2010

Associate Professor of Chemical Engineering, June 2004 – June 2008

Assistant Professor of Chemical Engineering, August 1999 – June 2004

Graduate Program Coordinator, March 2008 – May 2010

Distinguished Faculty Fellow, Sept 2007 – Sept. 2008

Undergraduate Program Coordinator, January 2003 to March 2008

Cookeville, TN

University of Tennessee – Space Institute

Adjunct Associate Professor of Chemical Engineering, July 2004 to December 2010

Tullahoma, TN

Sandia National Laboratories

University Summer Faculty Program (New Initiatives), Summer 2001

Livermore, CA

University Summer Faculty Program (Computational Biology), Summer 2000

Albuquerque, NM

AlliedSignal, Inc.

Research Engineer, May 1996 – December 1996
Fluorine Products Division, Buffalo NY

US Navy

Officer Student, Nuclear Propulsion Program, June 1992 – June 1994
Newport RI, Orlando FL, Ballston Spa NY

Union Carbide Corporation

Engineering Intern, June 1991 – August 1991
Seadrift TX

Honors and Awards

- Service to Chemical Engineering Education, AIChE, 2017
- Fellow, ASEE, 2015
- Stephen Brunauer Award, ACerS Cements Division, 2015
- Neva Gibbons Lectureship in Chemical Engineering Education, South Carolina, 2014
- Outstanding Graduate Student Faculty Mentor, UASIS, 2012
- Joseph J. Martin Award, ASEE (National Chemical Engineering Division), 2011
- ASEE PIC V, Outstanding Paper Award, 2010
- National Outstanding Teaching Award, ASEE, 2009
- Outstanding Teaching Award, ASEE-SE, 2008
- Distinguished Faculty Fellow (Tenn. Tech). 2007
- Outstanding Faculty Award in Teaching (Tenn. Tech), 2007
- ASEE Zone 2 Outstanding Campus Representative 2007
- ASEE-SE Outstanding Campus Representative 2007
- Ray E. Fahien Award, ASEE (National Chemical Engineering Division), 2006
- Brown-Henderson Outstanding Engineering Faculty Award (Tenn. Tech), 2006
- Leighton E. Sissom Innovation and Creativity Award (Tenn. Tech), 2006
- ASEE-SE New Faculty Research Award (1st Place), 2005
- Presidential Early Career Scientist and Engineer Award (PECASE), 2004
- NNSA DOE-DP Early Career Scientist and Engineer Award, 2004
- ASEE-SE Outstanding Campus Representative (2nd Place), 2004
- ASEE-SE New Faculty Research Award (2nd Place), 2003
- Sigma Xi Research Award (Tenn. Tech.), 2002
- ASEE Membership Award (SE Section), 2001
- Kinslow Engineering Research Award (Tenn. Tech.), 2000
- NSF Engineering Education Scholar, 1998
- DOE Graduate Assistantship in Areas of National Need (GAANN) Fellow, 1998
- Outstanding Teaching-Service Award (Buffalo) 1998,1999
- Letter of Commendation, United States Navy, 1993
- Engineer-in-Training (passed F.E. exam, NY state), 1992
- Graduated *cum laude*, 1992
- Outstanding Senior Student, American Institute of Chemists, 1992
- Academic Council Club of the Year, NSPE (Chapter President), 1992
- Western NY Student of the Year, AIChE, 1991
- Tau Beta Pi, 1991

Refereed Journal Publications (proceedings are *not* listed)

1. K. Koskey, N. Makki, W. Ahmed, H. Garafolo, D. Visco and B. Kruggel, "A Validity Study Applying the Rasch Model to the American Association for the Advancement of Science Force and Motion Sub-Topic Assessment for Middle School Students", *J. Applied Measurements*, In Press (2019).
2. Chen, J. J. F. Schmucker, L. N., and Visco, D. P. "Virtual high-throughput screens identifying hPK-M2 inhibitors: Exploration of model extrapolation", *Computational Biology and Chemistry*, **78**, 317 (2019).
3. Chen, J. J. F. Schmucker, L. N., and Visco, D. P. "Identifying De-NEDDylation Inhibitors: Virtual High-Throughput Screens Targeting SENP8", *Chemical Biology and Drug Design*, **93**, 590 (2019).
4. Chen, J. J. F. Schmucker, L. N., and Visco, D. P. "Identifying New Clotting Factor XIa Inhibitors in Virtual High-Throughput Screening Using PCA-GA-SVM Models and Signature", *Biotechnology Progress*, **34**, 1553 (2018).
5. Chen, J. J. F. Schmucker, L. N., and Visco, D. P. "Pharmaceutical Machine Learning: Virtual High-Throughput Screens Identifying Promising and Economical Small Molecule Inhibitors of Complement Factor C1s", *Biomolecules*, **8**, 51 (2018).
6. N. Garafolo, N. Makki, K. Halasa, W. Ahmed, K. Koskey and D. P. Visco, Jr. "Exploring the Engineering Design Process Through Computer-Aided Design and 3-D Printing", *Science Scope*, **41**, 51 (2017).
7. J. Chen and D. Visco, Jr. "Identifying Novel Factor XIIIa inhibitors with PCA-GA-SVM developed vHTS models", *Eur. J. Med. Chem.* **140**, 31 – 41 (2017).
8. J. Chen and D. Visco, Jr. "Developing an *in silico* pipeline for faster drug candidate discovery: Virtual high throughput screening with the Signature molecular descriptor using support vector machine models", *Chem Eng Sci*, **159**, 31 – 42 (2017).
9. D. P. Visco, Jr. "Teaching Tips: Approach Teaching Using Research Skills", *Chem. Eng. Ed.*, **48**, 250 (2014).
10. H. Li, D. P. Visco, Jr. and N. Leipzig, "Confirmation of Predicted Activity for Factor XIa Inhibitors from a Virtual High-Throughput-Screening Approach", *AIChE J*, **60**, 2741 - 2746 (2014).
11. N. Shlonimskaya, J. Biernacki, H. Kayello and D. P. Visco, Jr. "An Application of Computer-Aided Molecular Design (CAMD) Using the Signature Molecular Descriptor – Part 2: Evaluating newly identified surface tension reducing substances for potential use a shrinkage reducing admixtures", *Journal of the American Ceramic Society*, **97**, 378 – 385 (2014).
12. H. Kayello, N. Tadisina, N. Shlonimskaya, J. Biernacki and D. P. Visco, Jr. "An Application of Computer-Aided Molecular Design (CAMD) Using the Signature Molecular Descriptor – Part 1: Identification of Surface Tension Reducing Agents and the Search for Shrinkage Reducing Admixtures", *Journal of the American Ceramic Society*, **97**, 365 – 377 (2014).

13. B. Baburao and D. P. Visco, Jr. "Methodology for the Development of Thermodynamic Models Describing Substances that Exhibit Complex Association Patterns", *Ind. Eng. Chem. Res.*, **56**, 1506 – 1525 (2011).
14. J. Keith, D. P. Visco, Jr. D. L. Silverstein, and L. Bullard "Ideas to Consider for New Chemical Engineering Educators: Part 2 (Courses Offered Later in the Curriculum)" *Chem. Eng. Ed.*, **44**, 306 – 317 and 298 (2010).
15. P. Kannan, J. Biernacki, D. P. Visco, Jr., J. Dunne , A. Methner and D. Kirby, "Gas Diffusion Through EPS Foam", *J. Cell. Plas*, **46**, 353 – 373 (2010).
16. D. Weis and D. P. Visco, Jr. "Computer-Aided Molecular Design Using the Signature Molecular Descriptor: Application to Solvent Selection", *Comput. & Chem. Eng.*, **34**, 1018 – 1029 (2010)
17. P. Kannan, J. Biernacki and D. P. Visco, Jr. "Fast Pyrolysis Kinetics of Expanded Polystyrene Foam", *AIChE J*, **56**, 1569 - 1577 (2009).
18. P. Kannan, J. Biernacki, D. P. Visco, Jr. and W. Lambert, "Kinetics of Thermal Decomposition of Expanded Polystyrene in Different Gaseous Environments", *J. of Analytical and Applied Pyrolysis*, **84**, 139 – 144 (2009).
19. J. Keith, D. Silverstein and D. P. Visco, Jr. "Ideas to Consider for New Chemical Engineering Educators: Part 1 (Courses Offered Earlier in the Curriculum)", *Chem. Eng. Ed.*, **43**, 207 – 215 (2009).
20. S. Yelisetty and D. P. Visco, Jr., "Solubility of HFC32, HFC125, HFC152a, and HFC143a in Three Polyols", *J. Chem. Eng. Data*, **54**, 781 – 785 (2009).
21. A. Lucia, L. Octavio and D. P. Visco, Jr. "Modeling Association in the SAFT Formalism", *Comput. & Chem. Eng.*, **33**, 531 – 533 (2009).
22. J. Jackson, D. Weis and D. P. Visco, Jr., "Potential Glucocorticoid Receptor Ligands with Pulmonary Selectivity using I-QSAR with the Signature Molecular Descriptor", *Chem. Bio. & Drug Design*, **72**, 540 – 550 (2008)
23. D. Weis, D. P. Visco, Jr. and J. L. Faulon, "Data Mining PubChem Using a Support Vector Machine with the Signature Molecular Descriptor: Classification of Factor X1a Inhibitors", *J. Molec. Graph. & Model*, **27**, 466 – 475 (2008).
24. B. Baburao and D. P. Visco, Jr., "Association Based Equation of State for Substances Forming Monomers, Dimers and Trimers", *Fluid Phase Equilibria*, **265**, 7 – 11 (2008).
25. B. Baburao. D. P. Visco, Jr. and T. Albu, "Association Patterns in (HF)_m(H₂O)_n (m + n = 2-8) Clusters", *J. Physical Chemistry A*, **111**, 7940 – 7956 (2007).
26. S. Swaminathan, D. P. Visco, Jr. and S. Sen, "Detection of Shallow Inclusions in Closed-Packed Granular Beds using Mechanical Impulses", *Applied Phys. Lett.*, **90**, 154107/1 – 154107/3 (2007)
27. B. Baburao and D. P. Visco, Jr., "Isothermal Compressibility Maxima of Hydrogen Fluoride in the Super Critical and Super Heated Vapor Region", *J. Physical Chemistry B*, **110**, 26204 –26210 (2006)

28. P. Kannan, J. J. Biernacki and D. P. Visco, Jr., "A Review of Physical and Kinetic Models of Thermal Degradation of Expanded Polystyrene Foam and Their Application to the Lost Foam Casting Process", *J. Analytical and Applied Pyrolysis*, **78**, 162 – 171 (2006)
29. B. Baburao, S. Swaminathan and D. P. Visco, Jr., "Make Your Teaching Assistant a Co-Instructor", *Chem. Eng. Ed.* **40**, (2006).
30. D. Weis, J. L. Faulon, R. C. LeBorne and D. P. Visco, Jr., "The Signature Molecular Descriptor. 5. The Design of Hydrofluoroether Foam Blowing Agents Using Inverse-QSAR", *Ind. Eng. Chem. Res.*, **44**, 8883 – 8891 (2005)
31. S. Sen, T.R. Krishna Mohan, D. P. Visco, Jr., S. Swaminathan, A. Sokolow, E. Avalos and M. Nakagawa, "Using Mechanical Energy as a Probe for the Detection and Imaging of Shallow Buried Inclusions in Dry Granular Media", *Int. J. Mod. Phys. B.*, **19**, 1 – 23 (2005)
32. S. Dube and D. P. Visco, Jr., "A Survey of the Graduate Thermodynamics Course in Chemical Engineering Departments across the United States", *Chem. Eng. Ed.* **39**, 258 – 263 (2005).
33. V. Challa and D. P. Visco, Jr., "Evaluating the SAFT-VR and the Sanchez-Lacombe EOS for Modeling the Solubility of Blowing Agents in Polyols", *J. Cell. Plas.*, **41**, 563 – 588 (2005)
34. S. Swaminathan and D. P. Visco, Jr., "Thermodynamic Modeling of Refrigerants Using the Statistical Associating Fluid Theory with Variable Range (SAFT-VR). I: Pure Components", *Ind. Eng. Chem. Res.*, **44**, 4798 (2005)
35. S. Swaminathan and D. P. Visco, Jr., "Thermodynamic Modeling of Refrigerants Using the Statistical Associating Fluid Theory with Variable Range (SAFT-VR). II: Mixtures", *Ind. Eng. Chem. Res.* **44**, 4806 (2005)
36. D. P. Visco, Jr. S. Swaminathan, T.R. Krishna Mohan, A. Sokolow and S. Sen, "Impulse Penetration into Idealized Granular Beds: Behavior of Cumulative Surface Kinetic Energy", *Phys. Rev. E.*, **70**, 051306 (2004).
37. C. Churchwell, M. D. Rintoul, S. Martin, D. P. Visco, Jr., A. Kotu, R. S. Larson, L.O. Sillerud, D. C. Brown and J. L. Faulon, "The Signature Molecular Descriptor. 3. Inverse Quantitative Structure-Activity Relationship of ICAM-1 Inhibitory Peptides", *J Molecular Graphics and Modelling*, **22**, 263 – 273 (2004).
38. C. Payne-Smith and D. P. Visco, Jr. "Evaluating the Thermodynamic Consistency of Experimental Data for HF+H₂O at 101.325 kPa", *J. Chem. Eng. Data*, **49**, 306 – 310 (2004).
39. J. F. Faulon, D. P. Visco, Jr. and R. S. Pophale, "The Signature Molecular Descriptor. 1. Extended Valence Sequences vs. Topological Indices in QSAR and QSPR studies", *J. Chem. Inf. Comput. Sci.*, **43**, 707 – 720 (2003).
40. J. L. Faulon, C. Churchwell and D. P. Visco, Jr. "The Signature Molecular Descriptor. 2. Enumerating Molecules from Their Extended Valence Sequences", *J. Chem. Inf. Comput. Sci.* **43**, 721 – 734 (2003).
41. B. Baburao and D. P. Visco, Jr. "Thermodynamic Modeling of HF-mixtures Using a Modified AEOS Model", *Ind. Eng. Chem. Res.*, **41**, 4863-4872 (2002).

42. D.P. Visco, Jr., R. S. Pophale, M. D. Rintoul and J. L. Faulon, "Developing a Methodology for an Inverse Quantitative Structure-Activity Relationship Using the Signature Molecular Descriptor", *J Molecular Graphics and Modelling*, **20**, 429 - 438 (2002).
43. J. P. Russum and D.P. Visco, Jr., "The Use of an Integration Technique to Trace Phase Equilibria Curves", *Chem. Eng. Ed.*, **36**, 134 – 137 (2002).
44. Galindo, S. J. Burton, G. Jackson, D. P. Visco and D. A. Kofke, "Improved Models for the Phase Behavior of Hydrogen Fluoride: Chain and Ring Aggregates in the SAFT approach and the AEOS Model", *Molec. Phys.*, **100**, 2241 – 2259 (2002)
45. D. P. Visco, Jr. and A. N. Cartwright, "A New Model for ASEE Student Chapters", *J. Eng. Ed.*, October 2001, 641 – 643.
46. D. P. Visco, Jr. and S. Sen, "Relaxation of Classical Particles in Two-Dimensional Anharmonic Single Well Potentials", *Phys. Rev. E*, **63**:021114 (2001).
47. D. P. Visco, Jr. and D. A. Kofke, "Improved Thermodynamic Equation of State for Hydrogen Fluoride", *Ind. Eng. Chem. Res.*, **38**, 4125 (1999).
48. D. P. Visco, Jr. and D. A. Kofke, "Modeling the Monte Carlo Simulation of Associating Fluids", *J. Chem. Phys.*, **110**, 5493 (1999).
49. D. P. Visco, Jr. and D. A. Kofke, "A Comparison of Molecular-Based Models to Determine Vapor-Liquid Phase Coexistence in Hydrogen Fluoride", *Fluid Phase Equil.*, **158-160**, 37 (1999).
50. D. P. Visco, Jr. and D. A. Kofke, "Vapor-Liquid Equilibria and Heat Effects of Hydrogen Fluoride from Molecular Simulation", *J. Chem. Phys.*, **109**, 4015 (1998).
51. D. P. Visco, Jr. and S. Sen, "A Study of the Dynamics of a Non-linear Oscillator which is Coupled to Various Heat Bath Models", *Phys. Rev. E.*, **58**, 1419 (1998).
52. D. P. Visco, Jr., E. Juwono and D. A. Kofke, "Heat Effects of Hydrogen Fluoride from Two Thermodynamic Models", *Int. J. of Thermophys.*, **19**, 1111 (1998).
53. D. P. Visco, Jr. and S. Sen, "Dynamics of an Anharmonic Oscillator which is Harmonically Coupled to a Many Body System and the Notion of an Appropriate Heat Bath", *Phys. Rev. E*, **57**, 224 (1998).
54. D. P. Visco, Jr., D. A. Kofke, and R. R. Singh, "Thermal Properties of Hydrogen Fluoride from EOS + Association Model", *AIChE J.*, **43**, 2381 (1997).

Book Chapters

1. D. P. Visco, Jr. and J. J. Chen, "Ch. 11. The Signature Molecular Descriptor in Molecular Design: Past and Current Applications", *Tools for Chemical Product Design*, Elsevier (2016).
2. D. P. Visco, Jr., "Chapter 9: Computer-Aided Molecular Design Algorithms", *Handbook of Cheminformatic Algorithms*, CRC Press (2010).

3. J. L. Faulon, D. P. Visco, Jr. and D. Roe, "Enumerating Molecules", Reviews in Computational Chemistry, Vol. 21, John Wiley and Sons, (2005).
4. F. A. Shutov and D. P. Visco, Jr. "Chapter 17: Blowing Agents for Polymer Foams", Hand Book of Polymeric Foams and Foam Technology (2nd Edition), Hanser Publishers, New York (2004).

Books

1. K. Dahm and D. P. Visco, Jr., Fundamentals of Chemical Engineering Thermodynamics, Cengage, 2014.

Books/Journals Edited

1. D. P. Visco, Jr. and P. Wankat, Startup: A Collection of Important CEE Papers on Teaching for New Faculty, *Chemical Engineering Education*, 2014. (Virtual Issue)

Patents

1. J. Biernacki, H. Kayello and D. P. Visco, Shrinkage Reducing Admixtures for Portland Cement Concrete, US Patent Filed 62/040,716 (August 2014)
2. J. Biernacki, H. Kayello and D. P. Visco, Shrinkage Reducing Admixture for Concrete, US Patent Filed 61/868,918 (August 2013)

Book Review

1. D. P. Visco, Jr., Teaching and Learning in STEM: A Practical Guide (Felder and Brent), in *Chemical Engineering Education*, **51**, 74 (2017)
2. D. P. Visco, Jr., Teaching Engineering, 2nd Edition (Wankat and Oreovicz), in *Chemical Engineering Education*, **50**, 97 (2016)

Proceedings

1. E. Wain-Weiss, N. Makki and D. Visco, "A Doctoral Teaching Program in Engineering at The University of Akron", ASEE Annual Meeting and Exposition Proceedings, 2018.
2. K. Koskey, W. Ahmed, N. Makki, N. Garafolo, B. Kruggel and D. Visco, "Zipping to STEM: Integrating Engineering Design in Middle School Science", ASEE Annual Meeting and Exposition Proceedings, 2018.
3. K. Koskey, N. Garafolo, N. Makki, W. Ahmed, D. Visco and U. Samreddy, "WIP: Validity and Reliability Testing of the Engineering Concept Assessment Modified for Eighth Grade", ASEE Annual Meeting and Exposition Proceedings, 2017.

4. N. Makki, N. Garafolo, W. Ahmed, K. Koskey, D. Visco and K. Halasa, "Integrating Engineering Design using CAD Software with Force and Motion Concepts in Middle School", ASEE Annual Meeting and Exposition Proceedings, 2017.
5. D. P. Visco and D. Schaefer, "Training Engineering Faculty to be Educators", ASEE Annual Meeting and Exposition Proceedings, 2015.
6. J. J. Biernacki, D. P. Visco, Jr., and H. M. Kayello, "Computer aided molecular design – A course-grain tool for accelerating discovery of molecular interactions with cement," Proceedings of the International US-Poland Workshop on Multiscale Computational Modeling of Cementitious Materials, ,Krakow, Poland., Krakow University of Technology, 2012.
7. T. Utschig, D. Schaefer and D. Visco, "A Proposed Teaching and Learning Curriculum for COMPLETEE Based on Current National Trends", Frontiers in Education Conference, 2012
8. J. J. Biernacki, D. P. Visco, E. Thurber and R. Pavlovsky, "Using Web Applets to Simulate Learning", ASEE Annual Meeting and Exposition Proceedings, 2011.
9. D. P. Visco, "Student Designed Desktop Modules in a Thermodynamics Course", ASEE Annual Meeting and Exposition Proceedings, 2011.
10. L. Bullard, D. P. Visco, D. L. Silverstein and J. M. Keith, "Strategies for Creating and Sustaining a Departmental Culture", ASEE Annual Meeting and Exposition Proceedings, 2010.
11. D. L. Silverstein, M. Vigeant, D. P. Visco and D. Woods, "How We Teach: Freshman Instruction in Chemical Engineering", ASEE Annual Meeting and Exposition Proceedings, 2010.
12. D. Schaefer, D. P. Visco, Jr. T. Utschig, J. P. Mohsen, N. Fortenberry, M. Prince and C. Finelli. "Preparing for Participation in SPEED – An ASEE Initiative for a Nationally Recognized Development Program for Engineering Educators", ASEE Annual Meeting and Exposition Proceedings, 2010.
13. T. Utschig, N. Fortenberry, J. P. Mohsen, D. Schaefer and D. P. Visco, Jr. "Strengthening the Performance of Engineering and Technology Educations Across the Discipline(SPEED)", ASEE Annual Meeting and Exposition Proceedings, 2009.
14. J. M. Keith, D. L. Silverstein and D. P. Visco, Jr. "Ideas to Consider for New Chemical Engineering Educators: Junior and Senior Level Courses", ASEE Annual Meeting and Exposition Proceedings, 2009
15. J. M. Keith, D. L. Silverstein and D. P. Visco, Jr. "Ideas to Consider for New Chemical Engineering Educators: Freshman and Sophomore Level Courses", ASEE Annual Meeting and Exposition Proceedings, 2008
16. D. P. Visco, Jr., A. Minerick and J. M. Keith, "Tips for New Faculty: Engaging Your Graduate Students in Independent Thought", ASEE Annual Meeting and Exposition Proceedings, 2007.
17. D. P. Visco, Jr., S. Swaminathan, L. Zagumny and H. Anthony, "Evaluation of Student Constructed Study Guides", ASEE Annual Meeting and Exposition Proceedings, 2007.

18. P. Arce and D.P. Visco, Jr., "A Freshman Course in Chemical Engineering: Merging First-Year Experiences with Discipline-Specific Needs", ASEE Annual Meeting and Exposition Proceedings, 2006.
19. B. Baburao, S. Swaminathan and D. P. Visco, Jr., "Graduate Students as Co-Instructor for an Undergraduate Course: Implementation and Assessment", ASEE Annual Meeting and Exposition Proceedings, 2006.
20. D. P. Visco, Jr., "Improving Your Evaluations by Demonstrating Concern for Your Students", ASEE Annual Meeting and Exposition Proceedings, 2004.
21. S. Sen, D. P. Visco, Jr. and T. R. Krishna Mohan, "Impulse Backscattering based Detection and Imaging of Shallow Buried Objects" in Granular Materials Based Technologies, Materials Research Society Symposium Proceedings, 2003.
22. S. Sen, S. Chakravarti, D. P. Visco, Jr, M. Nakagawa, J. Agui, Jr., and D. T. Wu, "Impulse Propagation in Granular Systems, Proceedings of PASI on Modern Challenges in Statistical Mechanics, American Inst of Physics Conference Proceedings, **658**, 357 – 379 (2003).
23. R. Parthasarathy and D. P. Visco, Jr., "Modeling the Solubility of Blowing Agents in Polyols", AIChE Annual Meeting Proceedings, 2002.

Invited Presentations

1. "A Call to Service", **AIChE Annual Meeting (Education Division Awards Session)**, Pittsburgh, PA; October 2018.
2. "Thoughts on Teaching Undergraduate Thermodynamics", **AIChE Annual Meeting**, Pittsburgh, PA; October 2018 (with K. Dahm).
3. "Training Engineering Faculty to be Effective Educators: History and Perspective", **Neva Gibbons Lecture – University of South Carolina**, October 2014.
4. "Strategies for Creating and Sustaining a Departmental Culture: Turning Theory into Action", **AIChE Annual Meeting (Best Papers from CEE and ASEE Proceedings)**, Pittsburgh, PA; November 2012 (with L. Bullard, D. Silverstein and J. Keith).
5. "Incorporating Educational Innovation into the Classroom", **NAE Frontiers of Engineering Education**, UC – Irvine, November 2011.
6. "Molecular Design using Signature," **Trine University**, September 2011.
7. "Computer-Aided Molecular Design: Approaches and Applications", **Georgia Institute of Technology**, Atlanta, GA; November 2009.
8. "Solving Inverse Molecular Design Problems Using the Signature Molecular Descriptor: Theory and Applications", **Rochester Institute of Technology**, Rochester, NY; May 2009.

9. "Solving Inverse Molecular Design Problems Using the Signature Molecular Descriptor: Theory and Applications", **Joint BioEnergy Institute**, Emery, CA; April 2009.
10. "Inverse Design Using Signature", **University of Rhode Island**, Providence, RI; May 2007.
11. "Young Faculty Forum: Perspectives on Tenure and Promotion", **AICHE Annual Meeting**, Cincinnati, OH; November 2005.
12. "The Signature Molecular Descriptor and its Role in Reverse Engineering", **University of Alabama**, Tuscaloosa, AL; September 2005.
13. "The Signature Molecular Descriptor: From QSAR Studies to Focused Database Design", **SIAM Computational Science and Engineering Conference**, Orlando, FL; February 2005.
14. "A Survey of Graduate Level Thermodynamics in the US", **AICHE Annual Meeting**, Austin, TX; November 2004. (with S. Dube).
15. "Solving the Inverse-QSAR Problem using the Signature Molecular Descriptor", **University at Buffalo, SUNY**, Buffalo, NY; October 2004.
16. "Solving the Inverse-QSAR Problem using the Signature Molecular Descriptor", **Vanderbilt University**, Nashville, TN; October 2004.
17. "Solving the Inverse-QSAR Problem using the Signature Molecular Descriptor", **University of Tennessee**, Knoxville, TN; September 2004.
18. "Exploring the Utility of the Signature Molecular Descriptor", **Sigma Xi Chapter Meeting**, Tennessee Technological University, Cookeville, TN; February 2004.
19. "Thermodynamic Modeling of Non-Ozone Depleting Polyurethane Foam Blowing Agents", **Honeywell, Inc.**, Buffalo, NY; March 2001.
20. "Thermodynamic Modeling of Non-Ozone Depleting Polyurethane Foam Blowing Agents", **Sigma Xi Chapter Meeting**, Tennessee Technological University, Cookeville, TN; January 2001.
21. "Thermodynamic and Molecular Modeling of Hydrogen Fluoride", **University of Nevada**, Reno, NV; May 1999.
22. "Thermodynamic and Molecular Modeling of Hydrogen Fluoride", **Illinois Institute of Technology**, Chicago, IL; March 1999.
23. "Thermodynamic and Molecular Modeling of Hydrogen Fluoride", **Michigan Technological University**, Houghton, MI; February 1999.

Workshops Facilitated

1. "From Syllabi and Grading Schemes, to Learning Outcomes, Classroom Scenarios and More – What You Need to Know", **The University of Akron New Faculty Learning Community**, Akron, OH; October 2018

2. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Pittsburgh, PA; October 2018. (with D. Silverstein and L. Bullard).
3. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Minneapolis, MN; October 2017. (with D. Silverstein and L. Bullard).
4. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, San Francisco, CA; November 2016. (with L. Bullard).
5. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Salt Lake City, UT; November 2015. (with D. Silverstein and L. Bullard).
6. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Atlanta, GA; November 2014. (with D. Silverstein and L. Bullard).
7. "New Faculty Workshop", ***University of Akron, College of Engineering***, January 2014.
8. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, San Francisco, CA; November 2013. (with D. Silverstein and L. Bullard).
9. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Pittsburgh, PA; October 2012. (with D. Silverstein and L. Bullard).
10. "Course-Specific Applications of Active Learning Techniques", ***ASEE ChE Division Summer School***, Bangor, ME; July 2012. (with D. Silverstein, L. Bullard and J. Keith)
11. "Development and Use of Hands-On, Experimental Modules in Any Classroom", ***ASEE ChE Division Summer School***, Bangor, ME; July 2012. (with A. Minerick, D. Thiessen and B. Van Wie)
12. "Effective Teaching for New or Prospective Faculty", ***AICHE Annual Meeting***, Salt Lake City, UT; November 2010. (with D. Silverstein and L. Bullard).
13. "New Ideas for Old Courses", ***ASEE ChE Division Summer School***, Pullman, WA; July 2007. (with D. Silverstein and J. Keith).
14. "New Teacher Workshop for Engineering and Science Faculty", ***Tennessee Technological University***, Cookeville, TN; August 2005.
15. "New Teacher Workshop for Engineering", ***Tennessee Technological University***, Cookeville, TN; August 2004.

Other Presentations

(§ Poster)

1. §“Zipping to STEM: Integrating Engineering Design in Middle School Science”, **American Society for Engineering Education Annual Meeting**, Salt Lake City, UT; June 2018 (with K. Koskey, W. Ahmed, N. Makki, N. Garafolo and B. Kruggel).
2. §“Virtual High-Throughput Screening Pipeline: Dataset Attribute Effects on Experimentally Validated Hit Rates”, **AICHE Annual Meeting**, Minneapolis, MN; October 2017 (with J. Chen and L. Schmucker).
3. §“Design of Corrosion Inhibitors in Concrete Pore Solution: Modelling and Experimentation”, **AICHE Annual Meeting**, San Francisco, CA; November 2016 (with S. P. Chinthala, O. Rosas, R. Gupta).
4. §“Virtual High-Throughput Screening Pipeline: Limitations, Characterizations and Applications to Different Targets”, **AICHE Annual Meeting**, San Francisco, CA; November 2016 (with J. Chen).
5. “Creating an in silico Drug Discovery Pipeline for Faster Drug Discovery”, **AICHE Annual Meeting**, Salt Lake City, UT; November 2015 (with J. Chen).
6. §“Computer Aided Search for Drug Candidates: Cathepsin-L”, **AICHE Annual Meeting**, Salt Lake City, UT; November 2015 (with J. Chen).
7. “An Application of Computer-Aided Molecular Design (CAMD) Using the Signature Molecular Descriptor: Designing New Water-Reducing Admixtures for Cement through Cement Paste Rheology Evaluation”, **AICHE Annual Meeting**, Atlanta, GA; November 2014 (with H. Kayello and J. Biernacki).
8. §“A Novel Computer-Aided Molecular Design Approach to Design New Non-Intuitive Chemical Admixtures for Cement”, **AICHE Annual Meeting**, Atlanta, GA; November 2014 (with H. Kayello, J. Biernacki, N. Shlonimskaya and O. Chaudhari).
9. §“Evaluating the Effect of Chemical Admixtures on the Rheological Properties of Fresh Cement Paste”, **AICHE Annual Meeting**, Atlanta, GA; November 2014 (with H. Kayello and J. Biernacki).
10. “A Novel Computer-Aided Molecular Design Approach to Design New Non-Intuitive Shrinkage Reducing Admixtures (SRAs) for Cement: A Modeling and Experimental Study for Improved Performance”, **AICHE Annual Meeting**, San Francisco, CA; November 2013 (with H. Kayello, J. Biernacki and N. Shlonimskaya).
11. “ChE Summer School Revisited: Course-Specific Applications of Active Learning Techniques”, **AICHE Annual Meeting**, San Francisco, CA; November 2013 (with L. Bullard, D. Silverstein and J. Keith).

12. "A Novel Computer-Aided Molecular Approach Using the Signature Molecular Descriptor to Design Potentially New Non-Intuitive Amyloid- β Aggregation Inhibitors", ***AICHe Annual Meeting***, San Francisco, CA; November 2013 (with H. Kayello, M. Moss, et al.).
13. §"Using an Integration Technique to Trace Coexistence Curves: Applications to Multi-Component Phase Equilibrium", ***AICHe Annual Meeting***, Pittsburgh, PA; November 2012 (with S. Magadi).
14. §"An Innovative Computer-Aided Molecular Design Approach to the Rational Design of Novel Small Molecular Inhibitors of Amyloid- β Aggregation", ***AICHe Annual Meeting***, Pittsburgh, PA; November 2012 (with H. Kayello, M. Moss, et al.).
15. "The Faculty Perspective on Student Interactions with Departmental Culture", ***AICHe Annual Meeting***, Salt Lake City, UT; November 2010 (with L. Bullard, D. Silverstein and J. Keith).
16. "Preparing for Participation in SPEED – An ASEE Initiative for a Nationally Recognized Development Program for Engineering Educators", ***American Society for Engineering Education Annual Meeting***, Louisville, KY; June 2010, (with D. Schaefer, T. Utschig, J. P. Mohsen, N. Fortenberry, M. Prince and C. Finelli).
17. "Strategies for Creating and Sustaining a Departmental Culture", ***American Society for Engineering Education Annual Meeting***, Louisville, KY; June 2010 (with L. Bullard, J. M. Keith and D. L. Silverstein)
18. §"CAMD with Signature: The Design of Environmentally-Friendly Solvents", ***AICHe Annual Meeting***, Nashville, TN; November 2009 (with D. Weis).
19. "Ideas to Consider for New Chemical Engineering Educators -- Junior and Senior Level Courses", ***AICHe Annual Meeting***, Nashville, TN; November 2009 (with J. M. Keith and D. L. Silverstein)
20. §"Design and Synthesis of Ionic Liquids for Use as Biomass Pre-Treatment", ***AICHe Annual Meeting***, Nashville, TN; November 2009 (with D. Weis).
21. "Ideas to Consider for New Chemical Engineering Educators: Junior and Senior Level Courses", ***American Society for Engineering Education Annual Meeting***, Austin, TX; June 2009 (with J. M. Keith and D. L. Silverstein)
22. "Learning to Design Experiments – An Integrated Approach", ***AICHe Annual Meeting***, Philadelphia, PA; November 2008 (with J. Biernacki, M. Oyanader, P. Arce and I. Carpen).
23. §"Experimentation and Modeling of Foam Blowing Agent Solubility in Polyols", ***AICHe Annual Meeting***, Philadelphia, PA; November 2008 (with S. Yelisetty)
24. "A Global Optimization-Quantum Chemistry Approach for a Predictive SAFT Equation for Mixtures", ***AICHe Annual Meeting***, Philadelphia, PA; November 2008 (with A. Lucia)
25. "Ideas to Consider for New Chemical Engineering Educators: Freshman and Sophomore Level Courses", ***AICHe Annual Meeting***, Philadelphia, PA; November 2008 (with J. M. Keith and D. L. Silverstein)
26. "The Inverse Design of Ionic Liquids for Pretreatment of Cellulose", ***AICHe Annual Meeting***, Philadelphia, PA; November 2008 (with D. Weis, B. Simmons and J. Faulon)

27. §“Data Mining PubChem with Signature: Prediction of Biological Activity for Small Molecules”, ***AIChE Annual Meeting***, Philadelphia, PA; November 2008 (with D. Weis, and J. Faulon)
28. §“Modeling Association in the SAFT Equation Using Ab Initio Quantum Chemistry”, ***AIChE Annual Meeting***, Philadelphia, PA; November 2008 (with A. Lucia, L. Octavio, E. Fileti and S. Canuto)
29. “Adding Hands-On Projects and Critical Thinking Exercises to a Thermodynamics Sequence”, ***American Society for Engineering Education Annual Meeting***, Pittsburgh, PA; June 2008
30. “Ideas to Consider for New Chemical Engineering Educators: Freshman and Sophomore Level Courses”, ***American Society for Engineering Education Annual Meeting***, Pittsburgh, PA; June 2008 (with J. M. Keith and D. L. Silverstein)
31. “Incorporating Projects and Problems in a Thermodynamics Course to Improve Critical Thinking/Real World Problem Solving”, ***American Society for Engineering Education—SE Section Meeting***, Memphis, TN; April 2008
32. “Thermodynamic Modeling of the Aqueous HF Mixture by Incorporating Self-and-Cross Association Interactions”, ***AIChE Annual Meeting***, Salt Lake City, UT; November 2007. (with B. Baburao)
33. “Incorporating Semester-Long Projects in Thermodynamics to Improve Critical Thinking/Real World Problem Solving”, ***AIChE Annual Meeting***, Salt Lake City, UT; November 2007.
34. §“Demonstrating the Effect of Multiple Sets of Parameters on Mixture Property Predictions for a SAFT-based EOS using Terrain Methodology”, ***AIChE Annual Meeting***, Salt Lake City, UT; November 2007 (with S. Swaminathan and A. Lucia).
35. §“Molecular Design of Trypsin Inhibitors using Signature”, ***AIChE Annual Meeting***, Salt Lake City, UT; November 2007 (with D. Weis, J. Faulon, S. Martin and S. Watowich).
36. §“Modeling and Experimentation of Polyol +Blowing Agent Systems”, ***AIChE Annual Meeting***, Salt Lake City, UT; November 2007 (with S. Yellisetty).
37. “Interpreting Student-Constructed Study Guides”, ***American Society for Engineering Education Annual Meeting***, Honolulu, HA; June 2007 (with H. Anthony, L. Zagumny and S. Swaminathan).
38. “Tips for New Faculty: Engaging Your Graduate Students in Independent Thought”, ***American Society for Engineering Education Annual Meeting***, Honolulu, HA; June 2007 (with A. Minerick and J. Keith).
39. “Evaluation of Student Constructed Study Guides”, ***American Society for Engineering Education—SE Section Meeting***, Louisville, KY; April 2007 (with S. Swaminathan, L. Zagumny and H. Anthony)
40. “Curricular Reform at Tennessee Tech”, ***AIChE Annual Meeting***, San Francisco, CA; November 2006 (with J. Biernacki and P. Arce).
41. “Diffusion in PS: A Multi-scale Approach”, ***AIChE Annual Meeting***, San Francisco, CA; November 2006 (with J. Biernacki and P. Kannan).

42. §“Gas Diffusion in PS Film”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with J. Biernacki and P. Kannan).
43. “A Hybrid Meta Density Functional Theory Study Examining the Association Patterns in (HF)_n/(H₂O)_m Clusters”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with B. Baburao and T. Albu).
44. “Design of a Freshman Chemical Engineering Course”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with P. Arce).
45. “Interpreting Student-Constructed Study Guides: A Constructivist/Constructionist Perspective”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with H. Anthony, L. Zagumny and S. Swaminathan).
46. §“Understanding the Phase Behavior of Aqueous Hydrogen Fluoride Mixtures by Incorporating Self and Cross-Associating Patterns”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with B. Baburao).
47. §“Evaluation of the Pure Component Parameterization Methodology on Mixture Property Predictions for Thermodynamic Equations of State Using Terrain Methods”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with A. Lucia and S. Swaminathan).
48. “The Isothermal Compressibility Peaks in Hydrogen Fluoride in the Super Critical and Super Heated Vapor Region”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with B. Baburao).
49. §“Inverse-QSAR for Inhibitors of Phosphate Cdc25b”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with D. Weis and J. Faulon).
50. “Design of New Cox-2 Inhibitors Using the Signature Molecular Descriptor”, **AICHE Annual Meeting**, San Francisco, CA; November 2006 (with D. Weis and J. Faulon).
51. “A Freshman Course in Chemical Engineering: Merging First-Year Experiences with Discipline-Specific Needs”, **American Society for Engineering Education Annual Meeting**, Chicago, IL; June 2006 (with P. Arce).
52. “Graduate Students as Co-Instructor for an Undergraduate Course: Implementation and Assessment”, **American Society for Engineering Education Annual Meeting**, Chicago, IL; June 2006 (with S. Swaminathan and B. Baburao).
53. “A Freshman Course in Chemical Engineering”, **American Society for Engineering Education—SE Section Meeting**, Tuscaloosa, AL; April 2006 (with P. Arce)
54. “Using Graduate Students to Teach an Undergraduate Class”, **American Society for Engineering Education—SE Section Meeting**, Tuscaloosa, AL; April 2006 (with B. Baburao and S. Swaminathan)
55. “Gas Diffusivity in Blown Polystyrene and Its Importance in the Lost Foam Casting Process”, **Tennessee Academy of Science Annual Meeting**, Martin; TN; November 2005. (with J. Platfoot, S. Schulz, W. McDonald, P. Kannan and J. Biernacki).
56. “Evaluation of the Integrate and Combined Methods in Mixture Phase Equilibrium Calculations Using Equations of State”, **AICHE Annual Meeting**, Cincinnati, OH; November 2005. (with S. Dube).

57. §“Incorporating Cross-Association in Aqueous Hydrogen Fluoride Mixtures”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with B. Baburao).
58. “A Graduate Student Inside an Undergraduate Classroom – An Integrated Experience”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with S. Swaminathan and B. Baburao).
59. §“Landmine Detection in Granular Beds: Behavior of Cumulative Surface Kinetic Energy”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with S. Swaminathan and S. Sen).
60. “Hydrogen Abstraction Reaction of Hydrofluorocarbons by the Hydroxyl Radical. A Hybrid Density Functional Theory with Specific Reaction Parameter Study”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with S. Swaminathan, S. Mikel and T. Albu).
61. §“Inverse-QSAR for Pharmaceutical Development Using the Signature Descriptor: Application to β -Secretase and COX-2 Inhibitors”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with D. Weis, J. Faulon, S. Martin and R. LeBorne).
62. §“Solving the Inverse-QSAR Problem with Signature Using a Reduced System”, ***AICHE Annual Meeting***, Cincinnati, OH; November 2005. (with D. Weis, J. Faulon, S. Martin and R. LeBorne).
63. “On the Heterogeneity of Graduate Level Thermodynamics Courses Offered in Chemical Engineering Programs in the United States”, ***American Society for Engineering Education Annual Meeting***, Portland, OR; June 2005 (with S. Dube).
64. “A Review of Course Management Issues for New Faculty: Options Available and Research Findings”, ***American Society for Engineering Education Annual Meeting***, Portland, OR; June 2005 (with A. Minerick).
65. “On the Heterogeneity of Graduate Level Thermodynamics Courses Offered in Chemical Engineering Programs in the United States”, ***American Society for Engineering Education—SE Section Meeting***, Chattanooga, TN; April 2005 (with S. Dube).
66. “A Review of Course Management Issues for New Faculty: Options Available and Research Findings”, ***American Society for Engineering Education—SE Section Meeting***, Chattanooga, TN; April 2005 (with A. Minerick).
67. “The Role of Cross-Association in Aqueous-HF Mixtures and its Effect on the Thermodynamic Properties”, ***Tennessee Academy of Science Annual Meeting***, Columbia; TN; November 2004. (with B. Baburao).
68. Effect of Pure Component Parameterization Procedures in Mixture Phase Predictions Via Equations of State”, ***Tennessee Academy of Science Annual Meeting***, Columbia; TN; November 2004. (with S. Swaminathan).
69. “Evaluation Of The Integrate Method in Mixture Phase Equilibrium Calculations Using Equations of State”, ***Tennessee Academy of Science Annual Meeting***, Columbia; TN; November 2004. (with S. Dube).
70. §“Modeling Polyol + Blowing Agent Mixtures Using The SAFT-VR EOS”, ***Tennessee Academy of Science Annual Meeting***, Columbia; TN; November 2004. (with V. Challa).

71. "Significance of Association Schemes in Modeling Aqueous Hydrogen Fluoride Mixtures", **AICHE Annual Meeting**, Austin, TX; November 2004. (with B. Baburao).
72. §"Thermodynamic Modeling of Various Refrigerants and Refrigerant Mixtures using Statistical Associating Fluid Theory with Variable Range (SAFT-VR)", **AICHE Annual Meeting**, Austin, TX; November 2004. (with S. Swaminathan).
73. "Exploring the Importance of Pure Component Parameterization Procedures in Predicting Mixture Phase Properties via Equations of State", **AICHE Annual Meeting**, Austin, TX; November 2004. (with S. Swaminathan).
74. §"The Effect of Signature Height on Information Content in Quantitative Structure Relationships", **AICHE Annual Meeting**, San Francisco, CA; November 2003. (with S. Martin, C. Churchwell and J. Faulon).
75. §"Inverse-QSPR for Compound Development Using The Signature Descriptor: Application to Hydrofluoroethers", **AICHE Annual Meeting**, San Francisco, CA; November 2003. (with D. Weis, C. Churchwell and J. Faulon).
76. "Improving Your Evaluations by Demonstrating Concern for Your Students", **AICHE Annual Meeting**, San Francisco, CA; November 2003.
77. "Thermodynamic Modeling of Aqueous-Hydrogen Fluoride Systems", **Tennessee Academy of Science Annual Meeting**, Franklin; TN; November 2003. (with B. Baburao).
78. "Developing Novel Hydrofluoroethers Using the Inverse-QSR Technique with Signature", **Tennessee Academy of Science Annual Meeting**, Franklin; TN; November 2003. (with D. Weis).
79. "Are Pure Component Parameterization Procedures Important in Mixture Property Prediction?", **Tennessee Academy of Science Annual Meeting**, Franklin; TN; November 2003. (with S. Swaminathan).
80. §"Insights to Phase Equilibrium Calculations via Equations of State", **Tennessee Academy of Science Annual Meeting**, Franklin; TN; November 2003. (with S. Dube).
81. "Evaluating the Information Content of a Newly Developed Molecular Descriptor", **Tennessee Academy of Science Annual Meeting**, Franklin; TN; November 2003.
82. "Probing Information Content in QSAR/Similarity Analyses using the Signature Molecular Descriptor", **ACS Annual Meeting**, New York, NY; September 2003. (with S. Martin, C. Churchwell and J. Faulon).
83. §"Examining the Consistency of Thermodynamic Data for Aqueous-HF at 1 Atm via Molecular Simulation and a Thermodynamic Model", **FOMMS 2003**, Keystone, CO; July 2003. (with C. Smith, D. Kofke and S. Wierzchowski).
84. "Phase Coexistence Evaluation through Integration", **American Society for Engineering Education—SE Section Meeting**, Macon, GA; April 2003 (with J. Russum).

85. "Modeling the Solubility of Blowing Agents in Polyols", **Tennessee Academy of Science Annual Meeting**, Johnson City; TN; November 2002. (with R. Parthasarathy).
86. "Evaluating of the Signature Molecular Descriptor in Compound Design and Library Screening", **Tennessee Academy of Science Annual Meeting**, Johnson City; TN; November 2002. (with J. L. Faulon, C. Churchwell and A. Kotu).
87. "SAFT-VR Modeling of PUR Blowing Agents and Mixtures", **Tennessee Academy of Science Annual Meeting**, Johnson City; TN; November 2002. (with S. Swaminathan).
88. "Molecular Simulation of R-245fa", **Tennessee Academy of Science Annual Meeting**, Johnson City; TN; November 2002. (with A. Narayanan).
89. "Modeling the Solubility of Blowing Agents in Polyols", **AIChE Annual Meeting**, Indianapolis, IN; November 2002. (with R. Parthasarathy).
90. "Evaluating of the Signature Molecular Descriptor in Compound Design and Library Screening", **AIChE Annual Meeting**, Indianapolis, IN; November 2002. (with J. L. Faulon, C. Churchwell and A. Kotu).
91. "The Use of an Integration Technique to Trace Coexistence Curves", **AIChE Annual Meeting**, Indianapolis, IN; November 2002.
92. "Evaluating the Thermodynamic Consistency of an Aqueous Hydrogen Fluoride System Using the SAFT-VR Model", **AIChE Annual Meeting**, Indianapolis, IN; November 2002. (with C. Payne-Smith)
93. "The Use of an Integration Technique to Trace Phase Equilibria Curves", **American Society for Engineering Education Annual Meeting**, Montreal, Quebec; June 2002 (with J. Russum).
94. "Controlling Degeneracy with the Extended Valence Sequence Signature Molecular Descriptor", **American Chemical Society National Meeting**, Orlando, FL; April 2002 (with J.L. Faulon and C. Churchwell).
95. "Analyzing the Thermodynamic Consistency of an HF-solution Using a Molecular-Based Model" **AIChE Regional Student Conference – Mid Atlantic**, Blacksburg, VA; March 2002. (with C. Payne-Smith)
96. "Thermodynamic Modeling of HF-mixtures Using a Modified AEOs", **AIChE Spring Meeting**, New Orleans, LA; March 2002. (with B. Baburao).
97. "Library Design Using Deterministic Inverse Imaging and a Universal Descriptor", **AIChE Annual Meeting**, Reno, NV; November 2001. (with J. L. Faulon and M. D. Rintoul).
98. "Thermodynamic Modeling of Hydrogen Fluoride Mixtures", **111th meeting of the Tennessee Academy of Science**, Murfreesboro, TN; November 2001 (with B. Baburao).
99. "Signatures as Descriptors in 2D QSAR", **111th meeting of the Tennessee Academy of Science**, Murfreesboro, TN; November 2001 (with R. S. Pophale).
100. "Library Design Using Deterministic Inverse Imaging", **American Chemical Society National Meeting**, San Diego, CA; April 2001 (with J.L. Faulon and M. D. Rintoul).

101. [§]"Thermodynamic Modeling of Polyurethane Foam Blowing Agents", *AIChE Annual Meeting*, Los Angeles, CA; November 2000.
102. "SAFT-VR for HFC Blowing Agents – Pure Components and Mixtures", *110th Meeting of the Tennessee Academy of Science*, Nashville, TN; November 2000.
103. "Setting Up a Student Chapter of ASEE at S.U.N.Y. at Buffalo", *American Society for Engineering Education Annual Meeting*, St. Louis, MO; June 2000 (with A. Cartwright and M. Saroka).
104. "A New Thermodynamic Model for Hydrogen Fluoride", *109th meeting of the Tennessee Academy of Science*, Memphis, TN; November 1999 (with D. A. Kofke)
105. "Molecular-Orbital Derived Potential for Hydrogen Fluoride", *AIChE Annual Meeting*, Dallas, TX; November 1999 (with S. Wierzchowski, J. Gao and D. A. Kofke).
106. "Thermodynamic Modeling of Hydrogen Fluoride", *Thermodynamics 99: Thermodynamics and Statistical Mechanics with Industrial Applications*, London, England; April 1999 (with D. A. Kofke).
107. "A Study of Intermolecular Potentials for Hydrogen Fluoride", *AIChE Annual Meeting*, Miami, FL; November 1998 (with D. A. Kofke).
108. [§]"Vapor-Liquid Equilibria and Heat Effects of Hydrogen Fluoride from Simulation", *Graduate Student Symposium, S.U.N.Y. at Buffalo*, Buffalo, NY; May 1998 (with D. A. Kofke).
109. [§]"Molecular Modeling of Hydrogen Fluoride", *Eighth International Conference on Properties and Phase Equilibria for Product and Process Design*, Noordwijkerhout, The Netherlands; April 1998 (with D. A. Kofke).
110. "Molecular and Thermodynamic Modeling of Hydrogen Fluoride", *Physical Chemistry-Chemical Engineering Seminar, S.U.N.Y. at Buffalo*, Buffalo, NY; February 1998.
111. "Molecular Modeling of Hydrogen Fluoride", *AIChE Annual Meeting*, Los Angeles, CA; November 1997 (with D. A. Kofke).
112. "Thermodynamic Modeling of Hydrogen Fluoride", *NIST Thirteenth Symposium on Thermophysical Properties*, Boulder, CO; June 1997 (with E. Juwono and D. A. Kofke).

Professional Activities

Professional Society Memberships and Officer/Leadership Positions

- ***American Institute of Chemical Engineers***
 - Education Division
 - Future Faculty Mentor Committee Chair (2016 – 2018)
 - Past Division Chair (2014 – 2016)
 - Awards Committee (2014 – 2015)
 - Division Chair (2012 – 2014)
 - 1st Vice Chair (2010 – 2012)
 - Group 4 (Education)
 - Vice Chair, Group 4 (2009 – 2010)
 - Chair, Area 4a (2008)
 - Vice Chair, Area 4a (2005 – 2007)

- ***American Society for Engineering Education***
 - Chemical Engineering Division
 - Summer School Organizing Committee (2012 – 2017)
 - Chair (2008)
 - Chair Elect (2007)
 - Co-Chair, Awards Committee (2006)
 - New Engineering Educators Division
 - Chair (2005)
 - Program Chair (2004)
 - Secretary (2003)
 - Southeastern Section
 - Chair, *Programs Unit* (2008)
 - Technical Program Chair, Sectional Annual Meeting (2007)
 - Chair, *Publications and Promotions Unit* (2006)
 - Secretary, *Programs Unit* (2006)
 - Vice-Chair, *Publications and Promotions Unit* (2005)
 - Secretary, *Publications and Promotions Unit* (2004)
 - Founding Chair, *Chemical Engineering Division* (2003,2004)
 - Program Chair, Chemical Engineering Division (2003, 2004)

 - University
 - University of Akron, Campus Representative (2011 – Present)
 - Tennessee Technological University, Campus Representative (2000 – 2011)
 - University at Buffalo Student Chapter, Founding Member (1998)

- ***Sigma Xi*** (TTU Chapter)
 - Past-President (2006 – 07)
 - President (2005 – 06)
 - President Elect (2004 – 05)

- ***Omega Chi Epsilon***
 - (*Faculty Advisor*) 2000 - 2004

Session Organizer

- Organized sessions for the following organizations at a variety of conferences and technical meetings:
 - AIChE Annual Meetings
 - Education Division, Area 1a, Area 4
 - ASEE Annual Meetings
 - Chemical Engineering Division, New Engineering Educator Division
 - ASEE – SE Section Annual Meetings
 - Chemical Engineering Division
 - Tennessee Academy of Sciences

Technical Reviewer

- *Industrial and Engineering Chemistry Research*
- *Fluid Phase Equilibria*
- *Thermochemica Acta*
- *Journal of Chemical and Engineering Data*
- *Journal of Chemical Information and Computer Science*
- *Chemical Engineering Education*
- National Science Foundation – Panel Reviewer
- American Chemical Society – Petroleum Research Fund
- ASEE Conference Proceedings (NEE Division and ChE Division)
- US-Israel Bi-National Science Foundation

Editorial Positions

- Editor, *Chemical Engineering Education* (2019 – Pre)
- Associate Editor, *Chemical Engineering Education* (2018 – 2019)
- Assistant Editor, *Chemical Engineering Education* (2016 – 2018)

Accreditation

- Serves as a program evaluator (PEV) for AIChE to ABET-EAC (2012 – present)

Grants Awarded (PI and co-PI)

- National Science Foundation, “*Zip to Industry: A First-Year Corporate-STEM Connection Program*” \$449,838 (9/17 – 9/20). **PI**
- Ohio Board of Regents, “*OMIC 4*” (\$30,000 State; \$30,000 Industry Match) (7/17 – 12/19). **PI**
- National Science Foundation, “*Zippering Towards STEM: Integrating Engineering Design into the Middle School Physical Science Curriculum*”, \$742,356 (9/15 – 9/19). **PI**

- Ohio Board of Regents, “OMIC at UA: Building Connections, Building Infrastructure, Building Success”, \$1,703,000 (\$831,000 State; \$872,000 Industry/Other Match) (6/14 – 6/16). **PI**
- National Science Foundation, “I-Corps: Shrinkage Reducing Admixture Business Development”, \$50,000 (1/14 – 6/15).
- National Science Foundation, “AIR Option 1: Technology Translation -- Computationally Designed Shrinkage Reducing Admixtures for Concrete”, \$171,000 (9/13 – 2/15).
- Ohio Board of Regents, “Replicating a Proven Model to Provide Experiential Opportunities for Student Success”, \$2,600,000 (\$932,000 State; \$1,668,000 Industry) (1/13 – 6/14). **PI**
- National Science Foundation, “STEP: Math Success for STEM Majors”, \$957,000 (5/10 – 6/14). Proposal preparation/writing and execution (first-year) prior to leaving TTU.
- National Science Foundation, “RUI: Controlling the Properties and Performance of Concrete Using Computer-Aided Molecular Design”, \$372,000 (8/09 – 7/13).
- Department of Energy, “PECASE: Developing Novel Scaffolds for Biological Molecules by Solving the I-QSAR Problem Using the Signature Molecular Descriptor”, \$250,000 [+ \$80,000 internal match] (10/04 – 10/09). **PI**
- SACS Quality Enhance Program Award, “Critical Thinking / Real-World Problem Solving in a Thermodynamics Course”, \$3000 (08/06 – 08/07). **PI**
- TTU Faculty Research Committee Grant, “The Development of an Approach to Determine Useful Blowing Agent + Polyol Mixtures for Polyurethane Foam: Experimentation and Modeling”, \$4000 (08/06 – 08/08). **PI**
- National Science Foundation, “RREE: Interpreting Student-Constructed Study Guides: A Constructivist/Constructionist Perspective”, \$2,000 (01/06 – 07/06). **PI**
- TTU Center for Manufacturing Research “Analysis of Parameterization Approaches for Equations of State”, \$80,000 (08/03 – 08/07). **PI**
- American Chemical Society – Petroleum Research Fund, “Evaluating the Thermodynamics Effects of Self and Cross-Clustering on Strongly Associating Systems”, \$80,000 (01/05 – 08/07). **PI**
- National Science Foundation, “The TTU Regional Undergraduate Research Center”, \$50,000 (08/04 – 01/07). **PI**
- Honeywell, Inc., “Thermodynamic Modeling of Polymer Foam”, \$120,000 (+ \$26,000 internal match) (01/02 – 01/03). **PI**
- TTU Faculty Research Committee Grant, “Exploring the Validity of a Bonding Volume Assumption within the Statistical Association Fluid Theory”, \$3000, (08/01 – 08/02). **PI**
- Department of Energy (through Sandia National Laboratories) “Inverse Design for Biological Microsensors”, \$150,000 (01/01 – 01/04). **PI**
- TTU Faculty Research Committee Grant, “Thermodynamic Modeling of 1,1,1,3,3-Pentafluoropropane (R-245fa)”, \$3000 (08/01 – 08/02). **PI**

Teaching Experience

Courses Taught (* -- graduate level)

- 4200:225 *Equilibrium Thermodynamics*; Spring 2013 – 16, 19.
- CHE 3010 *Chemical Engineering Thermodynamics I*; Summer 2004, Fall 2004 - 10
- CHE 3021 *Separations and Solution Thermodynamics*, Spring 2008 - 10
- *CHE 7420 *Multi-Scale Modeling and Simulation* (w/ J. Biernacki), Fall 2006.

- *CHE 7410 *Advanced Topics in Inverse Molecular Design*, Fall 2006
- CHE 1010 *Introduction to Chemical Engineering*; Fall 2005 - 2008
- *CHEME 531 *Adv. Chemical Engineering Thermodynamics*; Fall 2004, 2006 (UTSI)
- HON 1010 *Introduction to Honors*; Fall 2004 – 2007
- *CHE 7030 *Molecular Thermodynamics*; Spring 2002 - 2003
- *CHE 6010 *Advanced Chemical Engineering Thermodynamics*; Fall 2001- 05
- CHE 3020 *Chemical Engineering Thermodynamics II*; Spring 2001,2003 – 07
- *CHE 6810 *Directed Studies in Computational Thermodynamics*; Spring 2001
- *CHE 6530 *Process Optimization*; Spring 2000 -- 2002
- CHE 2010 *Introduction to Chemical Engineering Analysis*; Fall 1999 – 03
- CHE 4540 *Process Dynamics and Control*; Spring 2004, 2005
- *CHE 4510/5510 *Applied Math in Chemical Engineering*; Fall 1999 - 01
- CHE 2210 *Intro. to Process Measurements (Lab)*; Spring 2000,2002,2005,2006
- *CHE 6810 *Statistical Mechanics and Transport Processes*; Fall 1999
- CE 328 *Chemical Engineering Lab 2*; Spring 1997, 1998 (instructor at Buffalo)
- CE 327 *Chemical Engineering Laboratory 1*; Fall 1996 (instructor at Buffalo)

Students Supervised

Graduate

- P. Chinthala, “Corrosion Inhibitors for Concrete: Design and Experiment” (M.S. – **Spring 2019**)
- J. Chen, “*Exploring Virtual HTS Environments Using the Signature Molecular Descriptor*” (**Ph. D. – May 2018**)
- H. Kayello, “*Computer-Aided Molecular Design Using the Signature Molecular Descriptor: An Application to Design Novel Chemical Admixtures for Concrete*” (**Ph. D. – August 2014**)
- S. Magadi, “*Use of an Integrate Method to Trace Coexistence Curves: Application to Pure and Multi-Component Mixtures*” (**M.S. – August 2013**)
- D. Weis, “*Optimizing Inverse Design Techniques Using Signature*” (**Ph.D. – May 2010**)
- N. Tadisina, “*A Thermodynamic Study on the Surface Tension of Amines and Glycol Ethers and Their Solutions with Water*”, (**M. S. – December 2010**) [co-advised with J. Biernacki]
- S. Yelisetty, “*Experiment and Modeling of Polyol + Blowing Agent Mixtures*” (**M.S. – August 2008**)
- R. Patel, “*Chemical Database Screening using Signature*” (**M.S. – August 2008**)
- B. Baburao, “*Modeling of HF + Water Mixtures*” (**Ph. D. -- May 2007**)
- S. Swaminathan, “*Detailed Analysis of Pure Component Parameterization Methodology on Mixture Property Prediction*” (**Ph. D. –May 2007**)
- D. Weis, “*Using the Inverse-QSAR Technique in Drug Design for Alzheimer’s Disease*” (**M.S. – Dec 2005**)
- N. Qualls, “*Inverse Design of Inhibitors for Candida Albicans*”, (**M.S. –August 2005**)
- V. Challa, “*Polyol + Blowing Agent Mixture Modeling Using SAFT*” (**M.S. – May 2005**)
- S. Dube, “*Evaluation of Novel Methods for Use in Mixture Phase Equilibrium Calculations*” (**M. S. – May 2005**)

- A. Narayanan, “Molecular Simulation of R-245fa with Pentane” (M.S. – August 2003)
- S. Swaminathan, “SAFT-VR Modeling of Blowing Agents and Mixtures” (M.S. – August 2003)
- A. Kotu, “Similarity, Diversity and the Solution of the Inverse Problem in QSAR using Signature” (M.S. – May 2003)
- R. Parthasarathy, “Modeling the Solubility of Hydrofluorocarbon Blowing Agents in Polyols” (M.S. – December 2002)
- R. Pophale, “Signatures as Descriptors in 2D QSAR” (M.S. – May 2002)
- B. Baburao, “Thermodynamic Modeling of HF/HFC mixtures” (M.S. – May 2002)

Undergraduate

- L. Schmucker, “Experimental Confirmation of Predicted Inhibitors”, (2017-18)
- P. Bertke, “Comparing Signature to Group Contribution Methods”, (2016-17)
- C. McCowin, “Design of Corrosion Inhibitors”, (2014-15)
- L. Aichinger, “Using Signature in BLOSUM Matrices”, (2014-15)
- A. Meyers, “Determining the Solubility of Cellulose in Ionic Liquids”, (Fall 2008)
- B. Brady, “Experimental Testing of Trypsin Inhibitors”, (Fall 2008)
- A. Parkes, “Experimental Determination of the Solubility of Foam Blowing Agents in Polyols”, (Fall 2008)
- A. Blumberg, “Evaluation of a Numerical Integrate Method to Determine Phase Coexistence”, (Fall 2008)
- S. Wynne, “Evaluation of the Feasibility of an Analytic Integrate Method to Determine Phase Coexistence”, (Fall 2008)
- J. Jackson, “Drug Design with Signature: Applications to COX-2”, (Spring 2007; Fall, Spring 2008)
- C. Heckman, “Drug Design with Signature: Advanced techniques at higher signature heights”, (Spring 2007; Fall, Spring 2008)
- D. Kirby, “Modeling and Experimentation of Film/Foam Diffusion”, (Spring 2007) – co-advised with J. Biernacki.
- S. Schulz and J. Platfoot, “Modeling and Experimentation of Diffusion in Foams and Films” (Fall 2005)
- C. Childers, “I-QSAR Studies Using Signature on COX-2 Inhibitors” (Fall 2004, Spring 2005)
- R. Rawlings, “I-QSAR Studies Using Signature on DHFR Inhibitors” (Fall 2004, Spring, 2005)
- Jesse Easterling, “Validation of the SLEOS Model used for Polyols and Blowing Agents” (Summer 2004)
- D. Weis, “The Inverse-QSR Approach using Signature on the Design of Hydrofluoroethers” (Spring 2002)
- C. Payne-Smith, “Evaluating the Thermodynamic Consistency of an Aqueous-HF system” (Spring 2002)
- J. Russum, “Comparison of Direct Evaluation and Integration of Phase Equilibria Curves” (Spring 2001)

University Service

The University of Akron

- Goldwater Scholarship Campus Representative (2013 – 2018)
- Faculty Advisor, Engineering Student Council (2012 – 2017)
- Honors Advisory Committee (2016 – 2017)
- University Pathways Committee (2014 – 2016)
- Flexible Class Scheduling Discussion Group (2014 – 2016)
- Multi-Year Experience Committee (2014 – 2015)
- Retention Champion – College of Engineering (2013 – 2015)
- Enrollment Management Committee (2013 – 2016)
- Hot Topics Committee (2011 – 2015)
- First-Year Engineering Experience Committee (2013 – 2016)
- Admissions and Recruitment Committee (2011 – 2015)
- Engagement Committee (2011 – 2012)

Tennessee Technological University

- Student Computing Initiative Committee (2008 – 2011)
 - University-wide Undergraduate Research Committee (2008 – 2011)
 - ASEE Awards Nomination Committee, Chair (2007 – 2011)
 - Faculty Senate Member, Engineering (2006 -- 2011)
 - Academic Council Member (2006 -- 2011)
 - UNIV 1020 First Year Connections Committee (2006 -- 2011)
 - *Ad hoc* Classroom Response System Committee (2006 – 2011)
 - Window on the World Steering Committee (2005 – 2011)
 - College of Engineering Undergraduate Curriculum Committee (2005 – 2011)
 - STEM Advisory Board (2005 – 2011)
 - Engineering Scholarship Awards Program Committee (2002)
 - Steering Committee for Engineering Faculty Academy for Scholarship in Teaching (2002)
 - Science Fair Judge, Putnam County, TN (1999 – 2011)
 - FE Exam Review Sessions in Chemistry (2000 – 2006)
 - Faculty Advisor for the Newman Center (Catholic Campus Ministry) (2000 – 2004)
-