Chau-Chyun Chen

Jack Maddox Distinguished Chair in Engineering
Department of Chemical Engineering
Texas Tech University
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Education

Sc.D. in Chemical Engineering, Massachusetts Institute of Technology, 1980
Dissertation: *Computer Simulation of Chemical Processes with Electrolytes*
Thesis Advisor: Professor Lawrence B. Evans

M.S. in Chemical Engineering, Massachusetts Institute of Technology, 1977
Dissertation: *A Pellicular Immobilized Enzyme System for the Regeneration of Adenosine 5′-Triphosphate*
Thesis Advisor: Professor Clark K. Colton

B.S. in Chemistry, National Taiwan University, 1973

Professional Experience

Sept. 2013 – Texas Tech University, Department of Chemical Engineering
Jack Maddox Distinguished Chair in Engineering

1981 – June 2013 Aspen Technology, Inc., Burlington, MA

- Vice President of Technology (July 2006 to June 2013)
- Senior Technology Fellow (July 2005 to June 2006)
- Technology Fellow (Sept 2000 to June 2005)
- Business Director for Applied Physical Properties & Chemistries
- Vice President of Advanced Technology
- Vice President and Director of Applications Technology;
- Vice President (Aspen Plus® Electrolytes Manager);
- Principal Engineer (Aspen Plus® Electrolytes Manager);
- Senior Engineer
- Co-founder

1994 - 1995 Massachusetts Institute of Technology, BioProcess Engineering Center
Research Affiliate

1992 - 1993 Massachusetts Institute of Technology, BioProcess Engineering Center
Visiting Scientist

1980 - 1981 Massachusetts Institute of Technology, Energy Laboratory
Research Engineer, ASPEN (Advanced System for Process Engineering) Project

Selected Honors/Awards

Elected Fellow of American Association for the Advancement of Science, November 2018

Elected Fellow of American Institute of Chemical Engineers, November 2015

EPISTAR Lectureship, National Tsinghua University, Taiwan, 2009

Elected Member of the National Academy of Engineering, February 2005
- For contributions to molecular thermodynamics and process modeling technology for designing industrial processes with complex chemical systems.

Computing Practice Award, Computing and Systems Technology Division, AIChE, 2001. - For Outstanding Leadership and Contributions to Industrial Practice of Molecular Thermodynamics and Fundamental Process Modeling of Complex Chemical Systems with Electrolytes and with Polymers.

Ted Peterson Best Paper Award, Computing and Systems Technology Division, AIChE, 1984. - In recognition of his paper: C.C. Chen, H.I. Britt, J.F. Boston & L.B. Evans, "A Local Composition Model for Excess Gibbs Energy of Electrolyte Systems," AIChE Journal, 1982, 25, 599.

Professional Societies

American Chemical Society
American Institute of Chemical Engineers
American Association for the Advancement of Science
Texas Academy of Medicine, Engineering & Science
U.S. National Academy of Engineering

Professional Activities and Services

- O'Donnell Awards Engineering Subcommittee Chair, Academy of Medicine, Engineering & Science of Texas, 2018
- O'Donnell Awards Committee Member, Academy of Medicine, Engineering & Science of Texas, 2016 – 2018
- Editorial Advisory Board Member of *Journal of Chemical & Engineering Data*, 2017 – 2019
- Editorial Advisory Board Member of *Fluid Phase Equilibria*, 2001 –
- Board Member, ASME-AIChE Joint Committee of Thermophysical Properties, 2015 –
- Director, Fuel and Petrochemical Division, American Institute of Chemical Engineers (AIChE), 2015 – 2017
- Programming Chair, Fuels and Petrochemical Division (Area 16), AIChE Annual Meeting, 2017 – 2019

- Session Chair, "Poster Session: Fuels and Petrochemical Division," 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
- NSF Career proposal review panel, Process Systems, Reaction Engineering and Molecular Thermodynamics, CBET/ENG, 2018
- NSF Career proposal review panel, Process Systems, Reaction Engineering and Molecular Thermodynamics, CBET/ENG, 2017
- Advisory Board Member, Modeling & Computational Science, Savannah River National Laboratory, 2017
- Session Chair, "Unconventionals: Hydrogen and Fuel Cells," AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017
- Programming Co-Chair, Fuels and Petrochemical Division (Area 16), AIChE Annual Meeting, 2015 – 2017
- NSF Panel on Molecular Thermodynamics and Nanoscale Materials, Process Systems, Reaction Engineering and Molecular Thermodynamics, CBET/ENG, 2016
- Sustainable Alternative Separations (ALTSEP) Roadmap Workshop, ACS Green Chemistry Institute and AIChE, July 14-16, 2016
- Session Chair, "Alternative Fuels and Enabling Technologies I," AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016
- Session Chair, "Surfaces, Interfaces and Confinement 2," 14th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal, May 22-26, 2016
- International Advisory Board Member, 14th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal, May 22-26, 2016
- Board Member, Advisory Board of Science and Technology for the National Institute of Clean-and-Low-Carbon Energy, Shenhua Group, China, 2009 – 2016
- Scientific Advisory Committee Member, 8th US-China Joint Chemical Engineering Conference, Shanghai, China, October 12-15, 2015
- Board Member (Industrial Trustee, 2003-2013; Academic Trustee, 2013-2014), the Computer Aids for Chemical Engineering Education (CACHE) Corporation (Not-for-Profit), 2003 – 2014
- Session Chair, "How Computing Has Changed Chemical Engineering – Session in Honor of Professor Larry Evans 80th Birthday," AIChE Annual Meeting, 2014, Atlanta, GA.
- Scientific Advisory Committee Member, 7th US-China Joint Chemical Engineering Conference, Beijing, China, October 14-18, 2013
- International Advisory Board Member, 13th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Iguazu Falls, Argentina-Brazil, May 26-30, 2013
- Editorial Advisory Board Member of *Industrial & Engineering Chemistry Research*, 2011 – 2013
- Guest Editorial Advisory Board Member, Annual Review of Chemical and Biomolecular Engineering, 2012
- Scientific Advisory Committee Member, 6th US-China Joint Chemical Engineering Conference, Beijing, China, November 7-10, 2011
- Awards Committee Member, American Institute of Chemical Engineers (AIChE), 2006-2010

- International Organizing Committee Member, 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, China, May 16-21, 2010
- Chemical Engineering Peer Committee Member, National Academy of Engineering, 2007-2009
- Board Member, Chinese American Chemical Society, 2008 – 2009
- Board Member, New England American Chinese Professionals, 2007 – 2009
- Symposium Co-Chair, "Computer Simulation and Experimental Validation", 5th US-China Joint Chemical Engineering Conference, Beijing, China, October 13-16, 2009
- Scientific Advisory Committee Member, 5th US-China Joint Chemical Engineering Conference, Beijing, China, October 13-16, 2009
- Session Co-Chair, "Robust and Uncertain Systems", Foundation for Computer-Aided Process Design, Breckenridge, Colorado, June 7-12, 2009
- Session Chair, "Pharmaceuticals," 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Hersonissos, Crete, Greece, May 20-25, 2007
- Member, Benchmark and Non-Simulation Predictive Methods Task Force, Industrial Fluid Property Simulation Collective, 2007
- Chair, Technical Publication Task Force, Aspen Technology, Inc., 2006
- Chair, University Consortium Program, Aspen Technology, Inc., 2005
- Chair, Technical Ladder Panel Review Program, Aspen Technology, Inc., 2005
- Chair, Technical Achievement Award Program, Aspen Technology, Inc., 2004
- Member, Technical Ladder Council, Aspen Technology, Inc., 2003-2006
- Session Chair, AIChE National Meeting, 2004, New Orleans, LA, "Phase Equilibria and Fluid Properties of Polymers and Heavy Oils"
- Editorial Board Member of *Chinese Journal of Process Engineering*, 2001 – 2003
- Technology Management Team Member, Aspen Technology, Inc., 2003 – 2004
- Technology Advisory Board Member, Aspen Technology, Inc., 2001– 2002
- Representative of Aspen Technology, Inc. at the Council for Chemical Research, 2001–2002
- Track Chair, AspenWorld 2002, Washington D.C., "Enabling and Emerging Technologies"
- Session Chair, AspenWorld 2002, Washington D.C., "Impact of Biotechnology and Its Future Commercial Development"
- Session Chair, AspenWorld 2002, Washington D.C., "Simulation and Optimization: Polymers"
- Session Chair, AIChE Annual Meeting, 2000, Los Angeles, CA, "Thermophysical Properties and Phase Behavior"
- Session Chair, AspenWorld 2000, Orlando, FL, "Process Development & Design for Polymers"
- Management Representative of Aspen Technology, Inc. at the Design Institute of Physical Property Data of AIChE, 1992 – 2000
- Session Chair, AIChE Symposium, 1992, New Orleans, LA, "Thermophysical Properties for Industrial Process Design; B. Property Modeling and Applications"

TEACHING ACTIVITIES

Teaching

- Molecular Thermodynamics for Chemical Engineers (ChE 5381; 3 credits) (Spring 2014)
- Advanced Chemical Engineering Thermodynamics (ChE 5231; 3 credits) (Fall 2014; Fall 2015; Fall 2016; Fall 2017)

Undergraduate Student Research Supervised

- Matt Hansen (6/2014-5/2016; graduated)
- Matt Kovalski (4/2014-5/2016; graduated)
- Vitasta Jain (7/2018-)

Graduate Students Supervised

- Nguyen H. Nguyen (MS; 6/2014-12/2014; graduated)
- Jieying Wu (MS; 1/2015-12/2016; graduated)
- Md Rashedul Islam (PhD; 9/2013-8/2017; graduated)
- Meng Wang (PhD; 1/2014-12/2017; graduated)
- Benjamin Caudle (MS; 6/2016-5/2018; graduated)
- Nazir Hossain (PhD; 6/2014-8/2018; graduated)
- Ashwin Ravichandran (PhD; 1/2014-12/2018)
- Yifan Hao (PhD; 1/2014-12/2018)
- Rajasi Shukre (MS; 9/2016-)
- Yue Yu (PhD; 1/2014-)
- Soraya Honarparvar (PhD; 1/2014-)
- Sina Hassanjani Saravi (PhD; 1/2014-)
- Sheik Tanveer (PhD; 1/2014-)
- Toni Kirkes (PhD; 6/2014-)
- Harnoor Kaur (PhD; 1/2015-)
- Abedi Samira (PhD; 1/2015-)
- Hla Tun (PhD; 1/2016-)
- Yuan Li (PhD; 1/2016-)
- Pradeep Vyawahare (PhD; 6/2016-)
- Michael Seas (PhD; 9/2017-)
- Ishan Pandey (PhD; 9/2018-)

Postdoctoral Students Supervised

- Md Rashedul Islam (postdoc; 9/2017 to date)
- Cheng-Hsiu Yu (postdoc; 10/2016-10/2017)
- Sanjoy Bhattacharia (postdoc, 1/2014-12/2016)
- Ehsan Sheikholeslamzadeh (postdoc, 2/2014-10/2014)

PhD Thesis Committee

- Parham Mobed (Chemical Engineering, 1/2014-12/2016)
- Young Yu (Petroleum Engineering, 9/2015-5/2017)

- Brent Sherman (UT-Austin, Chemical Engineering, 5/2013-5/2016)
- Rozana Bari (Chemical Engineering, 1/2015-)

RESEARCH ACTIVITIES

Summary of Research Productivity (as of 11/24/2018)

- Google Scholar: 7071 total citations, h-index: 40, i10-index: 69
- Web of Science: 4463 total citations, h-index: 30
- Research Interests: 1) molecular thermodynamics, thermophysical properties and fluid phase equilibria, adsorption isotherms, process modeling and simulation; 2) petroleum crude characterization, flow assurance, hydraulic fracturing & flow-back fluids, 3) nuclear waste and e-waste processing; 4) pharmaceutical and energetic material solubility modeling; 5) CO_2 capture systems, desalination systems, energy storage systems

Patents and Pending Patents

1. C.-C. Chen, M.R. Islam, M. Wang, Y. Hao, "Apparatus and Computerized Method for Predicting Asphaltene Precipitation Based on Aggregation Thermodynamics," PCT/US2016/029539; International Publication Number: WO 2016/176313 A1, November 3, 2016; US Application No. 2018/0314806, November 1, 2018

2. C.-C. Chen, H. Tun, H. Kaur, "Method and System for Adsorbed Phase Activity Coefficients for Mixed-Gas Adsorption," U.S. Provisional Patent Application No. 62/750,165, Date of Filing: October 24, 2018

3. C.-C. Chen, H. Que, "Method of Characterizing Chemical Composition of Crude Oil for Petroleum Processing," **U.S. Patent No. 9,934,367 B2**, April 3, 2018

4. A. Ravichandran, R. Khare, C.-C. Chen, "Apparatus and Computerized Method for Predicting NRTL Binary Interaction Parameters from Molecular Simulations," U.S. Provisional Patent Application, Date of Filing: July 17, 2017

5. C.-C. Chen, M.R. Islam, "Apparatus and Computerized Method for Optimizing or Generating a Sigma Profile for a Molecule," PCT/US2015/030108, Date of Filing: May 11, 2015; U.S. Patent Publication No.: 2017/0083688-A1., March 23, 2017

6. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment Model," **U.S. Patent No. 8,666,675**, March 4, 2014

7. S. Wang, Y. Song, C.-C. Chen, "Extension of COSMO-SAC Solvation Model for Electrolytes," **U.S. Patent No. 8,660,831**, February 25, 2014

8. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment Model," **U.S. Patent No. 8,527,210**, September 3, 2013

9. L. Zong, S. Ramanathan, C.-C. Chen, "System and Method of Modeling Mono-Glycerides, Di-Glycerides and Triglycerides in Biodiesel Feedstock," **U.S. Patent No. 8,515,722,** August 20, 2013

10. C.-C. Chen, H. Que, "Method of Characterizing Chemical Composition of Crude Oil for Petroleum Processing," European Patent Application No.: 13702132.5-1559, August 19, 2013

11. C.-C. Chen, "Modeling Physical Properties of Chemical Mixtures and Articles of Use," **U.S. Patent No. 8,346,525 B2**, January 1, 2013

12. X. He, S. Anavi, C.-C. Chen, "Systems and Methods for Modeling of Crystallization Processes," **U.S. Patent No. 8,315,842**, November 20, 2012

13. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment," **C.N. Patent No. 101310282A**, April 25, 2012

14. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment Model," **U.S. Patent No. 8,082,136**, December 20, 2011

15. S. Wang, Y. Song, C.-C. Chen, "Extension of COSMO-SAC Solvation Model for Electrolytes," European Patent Application No.: 11773157.0-1951, Date of Filing: December 10, 2011. Priority: US/13.10.10/USP 392549

16. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment Model," **U.S. Patent No. 7,941,277**, May 10, 2011

17. C.-C. Chen, Y. Song, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment-Based Ionic Activity Coefficient Model," **U.S. Patent No. 7,809,540 B2**, October 5, 2010

18. L. Zong, S. Ramanathan, C.-C. Chen, "System and Method of Modeling Mono-Glycerides, Di-Glycerides and Triglycerides in Biodiesel Feedstock," European Patent Office Application No. 10719478.9-2104 PCT/US2010032069, April 22, 2010

19. C.-C. Chen, Y. Song, "Methods of Modeling Physical Properties of Chemical Mixtures and Article of Use," **U.S. Patent No. 7,672,826 B2**, March 2, 2010

20. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment Model," European Patent Application No.: 06804184.7-1225, PCT/US2006/037601, Priority US/30.09.05/USA 241675, September 28, 2006

21. S. Treiber, S. Gorpade, A. Sirohi, S. Ramanathan, S. Lingard, C.-C. Chen, "Computer Method and Apparatus for Determining State of Physical Properties in a Chemical Process," **U.S. Patent No. 6,862,562**, March 1, 2005

22. S. Treiber, R. McLeod, A. Kalafatis, S. Ramanathan, S. Lingard, C.-C. Chen, "Computer Method and Apparatus for Optimized Controller in a Non-Linear Process," **U.S. Patent No. 6,654,649**, November 25, 2003

23. A.E. Hamielec, M. Osias, S. Ramanathan, A. Sirohi, C.-C. Chen, "Polymer Property Distribution Functions Methodology and Simulators," Japan Patent Pending, Attorney's Docket No.: 1086.1006-004

24. A.E. Hamielec, M. Osias, S. Ramanathan, A. Sirohi, C.-C. Chen, "Property Distribution Functions Methodology and Simulators," **European Patent No. 1070281**, July 3, 2002

25. A.E. Hamielec, M. Osias, S. Ramanathan, A. Sirohi, C.-C. Chen, "Polymer Property

Distribution Functions Methodology and Simulators," **U.S. Patent No. 6,093,211**, July 25, 2000

26. M. Barrera, G. Ko, M. Osias, S. Ramanthan, D.A. Tremblay, C.-C. Chen, "Polymer Component Characterization Method and Process Simulation Apparatus," **U.S. Patent No. 5,687,090**, November 11, 1997

Books

1. Thermophysical Properties for Industrial Process Design, co-editor with T. Selover, AIChE Symposium Series No. 298 (1994)

Manuscript in Preparation

1. Y. Yu, N. Hossain, **C.-C. Chen**, "Modeling of Polyelectrolytes System with Electrolyte Nonrandom Two-Liquid Model"

2. S. Tanveer, **C.-C. Chen**, "A Comprehensive Molecular Thermodynamic Model for the aqueous $Na^+-K^+-Ca^{2+}-Mg^{2+}-Cl^--SO_4^{2-}$ in High Salinity Produced Water"

3. M.R. Islam, **C.-C. Chen** "Aggregation thermodynamics of asphaltenes: prediction of precipitation in petroleum feedstock with NRTL-SAC"

4. Y. Hao, **C.-C. Chen**, "A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling"

5. N. Hossain, S.K. Bhattacharia, M. Haddix, **C.-C. Chen**, "Thermodynamic Solubility Modeling of 2,4,6-Trinitrotoluene (TNT)"

6. H. Tun, M. Haddix, **C.-C. Chen**, "Thermodynamic Solubility Modeling of 2, 2′, 4, 4′, 6, 6′ - Hexanitrostilbene (HNS)"

7. C.-H. Yu, **C.-C. Chen**, "A Modeling Methodology of Using Aspen Plus to Simulate CO2 Removal Efficiency in Rotating Packed Bed"

8. S. Abedi, N. Saturia, J. Hewitt, S.A. Vanapalli, **C.-C. Chen**, "Study of Solubility and Diffusivity of CO_2 in Aqueous NaCl Solutions Using Microfluidic Segmented Gas-Liquid Flows"

9. C.-K. Chang, **C.-C. Chen**, "Thermodynamic Langmuir Equation for Pure Component Isotherms"

10. B. Caudle, Y. Li, **C.-C. Chen**, "Thermodynamic Modeling of the Aqueous Copper(II) Nitrate and Aqueous Copper(II) Chloride Systems with Electrolyte-NRTL Model"

11. M. Wang, **C.-C. Chen**, "Predicting Wax Appearance Temperatures and Precipitation Profiles of Normal Alkane Systems: An Explicit Co-Crystal Model," to be submitted to *AIChE Journal* (2018)

12. N. Hossain, R. Islam, R. Khare, and **C.-C. Chen**, "Dissociation Behavior of Ionic Liquids in Solvents: Thermodynamic Modeling and Molecular Dynamics Simulation" to be submitted to *Journal of Chemical & Engineering Data* (2018)

Refereed Journal Articles

1. H. Kaur, H. Tun, M. Sees, **C.-C. Chen**, "Local Composition Activity Coefficient Model for Mixed-Gas Adsorption Equilibria," submitted to *AIChE Journal* (2018)

2. S. Honarparvar, **C.-C. Chen,** D. Reible, "Modeling Ion Transport in Electrodialysis of Concentrated Solutions," submitted to *Journal of Membrane Science* (2018)

3. S.H. Saravi, A. Ravichandran, R. Khare, **C.-C. Chen**, "Bridging Two-Liquid Theory with Molecular Simulations for Electrolytes: An Investigation of Aqueous NaCl Solution," in revision for *AIChE Journal* (2018)

4. S. Abedi, N.S. Suteria, **C.-C. Chen**, S.A. Vanapalli, "Microfluidic Production of Size-Tunable Hexadecane-in-Water Emulsions: Effect of Droplet Size on Destabilization of Two-Dimensional Emulsions due to Partial Coalescence," *Journal of Colloid and Interface Science* **533** (2019) 59-70

5. A. Ravichandran, **C.-C. Chen**, R. Khare, "Prediction of χ Parameter by Combining Molecular Simulations and Integral Equation Theory," *Journal of Physical Chemistry B.* **122** (2018) 9022-9031

6. N. Hossain, A. Ravichandran, R. Khare, **C.-C. Chen**, "Revisiting Electrolyte Thermodynamic Models: Insights from Molecular Simulations," *AIChE Journal* **64** (2018) 3728-3734

7. M.R. Islam, Y. Hao, **C.-C. Chen** "Thermodynamic Modeling of Asphaltene Precipitation in Pure and Mixed Solvents with NRTL-SAC," *Fluid Phase Equilibria* **473** (2018) 255-261

8. S.H. Saravi, S. Honarparvar, **C.-C. Chen** "Thermodynamic Modeling of HCl-H_2O Binary System with Symmetric Electrolyte NRTL Model," *Journal of Chemical Thermodynamics* **125** (2018) 159-171

9. A. Ravichandran, R. Khare, **C.-C. Chen**, "Predicting NRTL Binary Interaction Parameters from Molecular Simulations," *AIChE Journal* **64** (2018) 2758-2769

10. H. Kaur, M. Wang, M.B. Gorensek, **C.-C. Chen**, "Thermodynamic Modeling of the Hybrid Sulfur (HyS) Cycle for Hydrogen Production," *Fluid Phase Equilibria* **460** (2018) 175-188

11. S. Honarparvar, S.H. Saravi, D. Reible, **C.-C. Chen**, "Comprehensive Thermodynamic Modeling of Saline Water with Electrolyte NRTL Model: A Study of the Aqueous Sr^{2+}-Na^{+}-Cl^{-}-SO_4^{2-} Quaternary System," *Fluid Phase Equilibria*, **470** (2018) 221-231

12. M.R. Islam, Y.-F. Hao, M. Wang, **C.-C. Chen,** "Prediction of Asphaltene Precipitation in Organic Solvents via COSMO-SAC," *Energy and Fuels*, **31** (2017) 8985-8996.

13. M. Wang, H. Kaur, **C.-C. Chen**, "Thermodynamic Representation of Nitric Acid-Sulfuric Acid-Water Ternary System," *AIChE Journal*, **63** (2017) 3310-3317

14. S. Honarparvar, S.H. Saravi, D. Reible, **C.-C. Chen**, "Comprehensive Thermodynamic Modeling of Saline Water with Electrolyte NRTL Model: A Study on Aqueous Ba^{2+}-Na^{+}-Cl^{-}-SO_4^{2-} Quaternary System," *Fluid Phase Equilibria*, **447** (2017) 29-38

15. S. Tanveer, H. Zhou, **C.-C. Chen**, "Thermodynamic Modeling of Mg^{2+}-Na^{+}-K^{+}-Cl^{-} Quaternary System," *Fluid Phase Equilibria,* **437** (2017) 56-68

16. S.K. Bhattacharia, B.L. Weeks, **C.-C. Chen**, "Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX", *Journal of Chemical & Engineering Data,* **62** (2017) 967-972

17. M. Wang, Y.-F. Hao, M.R. Islam, **C.-C. Chen**, "Aggregation Thermodynamics for Asphaltene Precipitation", "Editor's Choice paper," *AIChE Journal*, **62** (2016) 1254-1264

18. N. Hossain, S.K. Bhattacharia, **C.-C. Chen**, "Temperature Dependence of Interaction Parameters in Electrolyte NRTL Model" *AIChE Journal*, **62** (2016) 1244-1253

19. N.H. Nguyen, F. Hussain, **C.-C. Chen**, "Correlations for Densities of Aqueous Electrolyte Solutions," *Journal of Chemical & Engineering Data*, **61** (2) (2016) 740-747

20. S. Tanveer, **C.-C. Chen**, "Thermodynamic Modeling of Ca^{2+}-Na^{+}-K^{+}-Cl^{-} Quaternary System," *Fluid Phase Equilibria*, **409** (2016) 193-206

21. M. Wang, M. Gorensek, **C.-C. Chen**, "Thermodynamic Representation of Aqueous Sodium Nitrate and Nitric Acid Solution with Electrolyte NRTL Model," *Fluid Phase Equilibria*, **407** (2016) 105-116

22. M. Wang, Y. Yu, **C.-C. Chen**, "Modeling Mixed Solvent Electrolytes," *Chemical Engineering Progress*, **112** (2) (2016) 34-42

23. R. Aguda, **C.-C. Chen**, "Solubility of Nutraceutical Compounds in Generally Recognized as Safe Solvents at 298 K," *International Journal of Chemical Engineering and Applications*, **7** (5) (2016) A721

24. M.R. Islam, **C.-C. Chen**, "COSMO-SAC Sigma Profile Generation with Conceptual Segment Concept," *Industrial & Engineering Chemistry Research*, **54** (2015) 4441-4454

25. S.K. Bhattacharia, S. Tanveer, N. Hossain, **C.-C. Chen**, "Thermodynamic Modeling of Na^{+}-K^{+}-Mg^{2+}-SO_4^{2-} Quaternary System," *Fluid Phase Equilibria*, **404** (2015) 141-149

26. S.K. Bhattacharia, N. Hossain, **C.-C. Chen**, "Thermodynamic Modeling of Na^{+}-K^{+}-Cl^{-}-SO_4^{2-} Quaternary System with Electrolyte NRTL Model," *Fluid Phase Equilibria*, **403** (2015) 1-9

27. S.K. Bhattacharia, **C.-C. Chen**, "Thermodynamic Modeling of KCl + H_2O and KCl + NaCl + H_2O Systems Using Symmetric Electrolyte NRTL Model," *Fluid Phase Equilibria*, **387** (2015) 169-177

28. S.H. Saravi, S. Honarparvar, **C.-C. Chen**, "Modeling Aqueous Electrolyte Systems," *Chemical Engineering Progress*, **111** (3) (2015) 65-75

29. S. Tanveer, Y.-F. Hao, **C.-C. Chen**, "Introduction to Solid-Fluid Equilibrium Modeling," *Chemical Engineering Progress*, **110** (9) (2014) 37-47

30. Y. Zhang, **C.-C. Chen**, "Modeling CO_2 Absorption and Desorption by Aqueous Monoethanolamine Solution with Aspen Rate-Based Model," *Energy Procedia*, **37** (2013) 1584-1596

31. E. Sheikholeslamzadeh, **C.-C. Chen**, S. Rohani "Optimal Solvent Screening for the

Crystallization of Pharmaceutical Molecules from Multi-Solvent Systems," *Industrial & Engineering Chemistry Research*, **51** (2012) 13792-13802

32. B. Hanley, **C.-C. Chen**, "New Mass Transfer Correlations for Packed Towers," *AIChE Journal*, **58**, (2012) 132-152 and 2290-2293

33. Y. Zhang, H. Que, **C.-C. Chen**, "Thermodynamic Modeling of CO_2 Absorption in Aqueous MEA Solution with Electrolyte NRTL Model," *Fluid Phase Equilibria*, **311** (2011) 68-76

34. H. Que, **C.-C. Chen**, "Thermodynamic Modeling of the NH_3-CO_2-H_2O System with Electrolyte NRTL Model," *Industrial & Engineering Chemistry Research*, **50** (2011) 11406-11421

35. M.D. Meixell, Jr., B. Gochenour, **C.-C. Chen**, "Industrial Applications of Plant-Wide Equation-Oriented Process Modeling - 2010," *Advances in Chemical Engineering*, **40** (2011) 119-152

36. L. Zong, **C.-C. Chen**, "Thermodynamic Modeling of CO_2 and H_2S Solubilities in Aqueous DIPA Solution, Aqueous Sulfolane-DIPA Solution, and Aqueous Sulfolane-MDEA Solution with Electrolyte NRTL Model," *Fluid Phase Equilibria*, **306** (2011) 190-203

37. Y. Yan, **C.-C. Chen**, "Thermodynamic Representation of the NaCl-Na_2SO_4-H_2O System with Electrolyte NRTL Model," *Fluid Phase Equilibria*, **306** (2011) 149-161

38. H. Que, Y. Song, **C.-C. Chen**, "Thermodynamic Modeling of the Sulfuric Acid-Water-Sulfur Trioxide System with the Symmetric Electrolyte NRTL Model," *Journal of Chemical and Engineering Data*, **56** (2011) 963-977

39. Y. Zhang, **C.-C. Chen**, "Modeling Gas Solubilities in Aqueous Methyldiethanolamine Solution," *Industrial & Engineering Chemistry Research*, **50** (2011) 6436-6446

40. S. Wang, Y. Song, **C.-C. Chen**, "Extension of COSMO-SAC Solvation Method for Electrolytes," *Industrial & Engineering Chemistry Research*, **50** (2011) 176-187

41. Y. Zhang, **C.-C. Chen**, "Thermodynamic Modeling of CO_2 Absorption in Aqueous Methyldiethanolamine Solution with Electrolyte NRTL Model," *Industrial & Engineering Chemistry Research*, **50** (2011) 163-175

42. Y. Yan, **C.-C. Chen**, "Thermodynamic Modeling of CO_2 Solubility in Aqueous Solutions of NaCl and Na_2SO_4," *Journal of Supercritical Fluids*, **55**, 623-634 (2010)

43. L. Zong, S. Ramanathan, **C.-C. Chen**, "Predicting Thermophysical Properties of Mono- and Diglycerides with the Chemical Constituent Fragment Approach," *Industrial & Engineering Chemistry Research*, **49** (2010) 5479-5484

44. L. Zong, S. Ramanathan, **C.-C. Chen**, "Fragment-Based Approach for Estimating Thermophysical Properties of Fats & Vegetable Oils for Modeling Biodiesel Production Processes," *Industrial & Engineering Chemistry Research*, **49** (2010) 876-886 and 3022-3023

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2. L. Zong, **C.-C. Chen**, "Development of a Segment-Based DEPG Physical Solvent Model for CO_2 Capture Processes," *Proceedings of 35th International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference")*, Clearwater, Florida, June 6-10, 2010
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Invited Lectures

1. *Recent Advances in Molecular Thermodynamics for Energy and Sustainability*, Lindsay Lecture Series, Department of Chemical Engineering, Texas A&M University, College Station, TX, September 12, 2018
2. *Electrolyte Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions*, Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan, March 29, 2018
3. *Modeling Best Practices Applied to RAPID Assessments*, Topical Conference: Process Intensification & Modular Chemical Processing, 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017.
4. *Recent Advances in Thermodynamic Modeling of Aqueous and Mixed Solvent Electrolyte Solutions*, 5th International Symposium on Aqua Science and Water Resources (ISASWR'17), Fukuoka University, Fukuoka, Japan, August 8-11, 2017.
5. *Perspectives in Thermodynamics Needs of Chemical Industry*, Department of Chemical Engineering, National Tsing-Hua University, Hsinchu, Taiwan, January 24, 2017
6. *Development of a Comprehensive Molecular Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions*, Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan, January 23, 2017
7. BIRS Workshop (16w5074): EPIC - Enabling Process Innovation through Computation, Banff, Canada, August 7-12, 2016
8. *Perspectives in Thermodynamics Needs of Chemical Industry*, Department of Chemical and Biomolecular Engineering, University of Houston, December 4, 2015
9. *Development of a Comprehensive Molecular Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions*, presented at the Session "In Honor of Stanley Sandler I", the 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
10. *Some Perspectives in Thermodynamics Needs of Chemical Industry*, presented at the Session "Thermodynamics Needs of Chemical Industry," the 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015

11. *Chemical Interactions of Mixed Waters*, presented at Workshop on Water Management – Utica and Marcellus Shale, Ohio State University, Cambridge, Ohio, June 10, 2015
12. *Why Advance Molecular Thermodynamic Models for Electrolyte Systems*, presented at the local AIChE section meeting, Aiken, SC., January 22, 2015
13. *Simulation-Based Science and Engineering with Energy and the Environment*, presented at 1° Taller Internacional Ingeniería y Energía: Conectando Ideas y Personas, Santiago, Chile, December 3-5, 2014
14. *The Role of Molecular Thermodynamics in Process Modeling,* invited lecture at the Session "How Computing Has Changed Chemical Engineering – Session in Honor of Professor Larry Evans' 80th Birthday," 2014 AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014
15. *Simulation-Based Science and Engineering with Conventional Energy*, invited area plenary lecture at the Session "Optimizing Health, Safety & Environmental (HSE) Sustainably," 2014 AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014
16. *Molecular Thermodynamic Model for Defense Waste Processing Facility Sludge Simulant*, invited lecture at SRNL Director's Colloquium, Aiken, SC, November 13, 2014
17. *Simulation-Based Science & Engineering for Sustainable Energy*, invited lecture at Enabling Process Innovation Through Computation (EPIC) Seminar Series, College of Engineering, Louisiana State University, Baton Rouge, LA, October 17, 2014
18. *Molecular Thermodynamics and Process Modeling Technology*, invited lecture at Seventh Joint China/USA Chemical Engineering Conference, Beijing, China, October 14-18, 2013
19. *Molecular Thermodynamics and Process Modeling Technology for Energy and the Environment*, Maddox Distinguished Lecture Series, Texas Tech University, Lubbock, Texas, September 25, 2012
20. *Molecular Thermodynamics and Process Modeling Technology for Energy and the Environment*, Graduate Student Lecture, Department of Chemical Engineering, Ohio State University, Columbus, Ohio, September 13, 2012
21. *Clean Energy Opportunities in Low Carbon Economy*, presented at University Centennial Industry Day Forum, Department of Chemical Engineering, National Tsing-Hua University, Hsinchu, Taiwan, April 15, 2011
22. *Process Modeling and Simulation for Energy and the Environment: An Industry Perspective*, Shenhua NICE Advisory Board Meeting, Pasadena, California, February 24-26, 2011
23. *Integrated, High Fidelity, Multiscale Process Models for the Process Industries*, presented at the topical conference on Simulation-Based Engineering and Science, AIChE Annual Meeting, Salt Lake City, Utah, November 7-12, 2010
24. *Opportunities and Challenges in Process Simulation and Applied Thermodynamics*, invited keynote lecture at the 13th Asian Pacific Confederation of Chemical Engineering Congress (APCChE 2010), Taipei, Taiwan, Oct 6-8, 2010
25. *Advances in Molecular Thermodynamics for Correlation and Prediction of Drug Molecule Solubility,* invited Chemical Engineering Colloquium lecture at University of Kentucky, Department of Chemical Engineering, April 28, 2010

26. *Process Modeling for the Changing World: From CO2 Capture to Drug Molecule Solubility*, invited Purdue School of Chemical Engineering Graduation Student Organization Seminar, Purdue University, April 6, 2010
27. *Molecular Thermodynamics for Pharmaceutical Product and Process Development*, invited lecture presentation at Fifth Joint China/USA Chemical Engineering Conference, Beijing, China, October 13-16, 2009
28. *Process Modeling and Simulation for Energy, the Environment and Medicine – An Industry Perspective*, Invited keynote lecture presentation at Process Design Symposium, 8th World Congress of Chemical Engineering, Montreal, Quebec, Canada, August 23-27, 2009
29. *A Journey of Learning in Process Modeling and Simulation*, EPISTAR lecture presentation at Chemical Engineering Department, National Tsinghua University, Taiwan, April 10, 2009
30. *Applied Thermodynamics for Process Modeling: History, Applications, Challenges and Opportunities,* EPISTAR lecture presentation at Chemical Engineering Department, National Tsinghua University, Taiwan, April 8, 2009
31. *Process Modeling and Simulation for Medicine, Energy and the Environment: A Focus on Modeling CO_2 Capture Processes*, EPISTAR lecture presentation at Chemical Engineering Department, National Tsinghua University, Taiwan, April 7, 2009
32. *Recent Advances in Correlation and Prediction of Drug Molecule Solubilities*, Invited Chemical Engineering Colloquium Lecture at Chemical Engineering Department, Worcester Polytechnic Institute, Worcester, Massachusetts, March 12, 2009
33. *Process Modeling and Simulation for Energy, the Environment and Medicine – An Industry Perspective*, Invited Chemical Engineering Colloquium Lecture at Chemical Engineering Department, University of Texas, Austin, Texas, February 17, 2009
34. *Recent Application Successes and Technology Advances in Process Modeling and Simulation for Product and Process Development*, paper presented at the PSE China Conference, Shanghai, China, September 19-21, 2008
35. *Recent Advances in Modeling and Simulation for Product and Process Development*, presented at the Chemical Engineering Department, Zhejiang University, Hangzhou, China, May 26, 2008
36. *Recent Advances in Modeling and Simulation for Product and Process Development*, presented at the Chemical Engineering Department, National Taiwan University, Taipei, Taiwan, April 3, 2008
37. *A Rate-Based Process Modeling Study of CO_2 Capture with Aspen RateSep*, Invited Lecture at McMaster University, Department of Chemical Engineering, Hamilton, Ontario, Canada, February 5, 2008
38. *A Rate-Based Process Modeling Study of CO_2 Capture with Aqueous MEA, MDEA and Activated TEA Solutions*, paper presented at the Chemical Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts, November 27, 2007

39. *High Impact Opportunities in Simulation-Based Product and Process* Development, paper presented at the U.S. Baseline Workshop on Simulation Based Engineering & Science, Arlington, VA, November 1-2, 2007
40. *Recent Advances in Modeling and Simulation for Product and Process Development*, paper presented at the PSE China Conference, Xian, China, August 15-18, 2007
41. *Modeling and Simulation for Pharmaceutical Product and Process Development*, with Bernard McGarvey, paper presented at the Workshop on Modeling Challenges in Process Development: Approaches in the Chemical and Pharmaceutical Industries, the Council for Chemical Research, University of Maryland Biotechnology Institute, Rockville, MD, June 7-8, 2007.
42. *Correlation and Prediction of Drug Molecule Solubility – Building the Molecular Thermodynamic Foundation for Pharmaceutical Process Modeling*, invited lecture at University of Notre Dame, Department of Chemical Engineering, South Bend, IN, March 21, 2007
43. *Correlation and Prediction of Drug Molecule Solubility – Building the Molecular Thermodynamic Foundation for Pharmaceutical Process Modeling*, Invited Chemical Engineering Colloquium Lecture at McMaster University, Department of Chemical Engineering, Hamilton, Ontario, Canada, March 8, 2007
44. *Correlation and Prediction of Drug Molecule Solubility with Molecular Thermodynamic Models – Building the Scientific Foundation for Pharmaceutical Process Modeling*, invited lecture at National Taiwan University, Department of Chemistry, Taipei, Taiwan, November 2, 2006
45. *Correlation and Prediction of Drug Molecule Solubility with Molecular Thermodynamic Models: Building the Scientific Foundation for Pharmaceutical Process Modeling*, Invited Chemical Engineering Colloquium Lecture at Virginia Polytechnic Institute and State University, Department of Chemical Engineering, Blacksburg, VA, October 23, 2006
46. *Modeling and Simulation in 2004: An Industrial Perspective*, with H. Britt, V. Mahalec, and A. McBrien, paper presented at FOCAPD 2004 (Foundations of Computer Aided Process Design), Princeton, NJ, July 11-16, 2004
47. *Polymer Process Modeling*, paper presented at BASF Symposium on Modeling and Simulation for Polymer Product and Process Development," Ludwigshafen, Germany, May 1997
48. *A Molecular Thermodynamic Model for Gibbs Energy of Mixing of Nonionic Surfactant Solutions,* paper presented at the 7th Congress of Asian Pacific Confederation of Chemical Engineers, Taipei, Taiwan, March 1996
49. *An Industrial Experience with Molecular Thermodynamics for Electrolyte Systems,* invited Chemical Engineering Colloquia lecture at University of California at Berkeley, Department of Chemical Engineering, May 7, 1990
50. *Industrial Applications of Process Simulators,* invited lecture at the Taipei International Chemical Industrial Show Conference, Taipei, Taiwan, August 25-30, 1989

51. *Some Recent Developments in Process Simulation for Reactive Chemical Systems,* invited lecture at 8th International Symposium on Solute-Solute-Solvent Interactions, Regensburg, Germany, 1987

Contributed Conference Presentations

2019

1. *Thermodynamic Modelling of Ca^{2+}-Na^{+}-Cl^{-}-CO_2 Quaternary System with Electrolyte NRTL Model*, with T. Chen, S. Honarparvar, D. Reible, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
2. *Modeling and Metrics Development for Biomass Pyrolysis Intensification via Autothermal Operation*, with B. Caudle, R. Shukre, M.B. Gorensek, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
3. *Modelling of Gas Separations By Pressure Swing Adsorption Using a Novel Steady-State Methodology*, with M. Sees, T. Kirkes, T. Kim, J. Scott, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
4. *Thermodynamic Modeling of Aqueous Multivalent Polyelectrolyte Systems with Polyelectrolyte NRTL Model*, with Y. Li, Y. Yu, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
5. *Correlation/Prediction of Swelling of Poly (N-isopropyl acrylamide) Hydrogels in Aqueous Solutions of NaCl Using Extended Enrtl Model*, with S. Tanveer, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
6. *Modeling Swelling Equilibrium of Sodium Polyacrylate in Water and Saline Water with Polyelectrolyte Non-Random Two Liquid Model*, with Y. Yu, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
7. *Thermodynamic Modeling of Lithium Salts with the Electrolyte NRTL Model Using Hydration Chemistry*, with T. Kirkes, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019
8. *Estimating the Thermophysical Properties of Black Liquor from Kraft Pulping*, with T. Kirkes, to be presented at 2019 AIChE Spring Meeting, New Orleans, LA, March 31-April 4, 2019

2018

9. *Steady-State Modeling of Air Separation by Pressure Swing Adsorption Using a Bed-State Efficiency Model,* with T. Kirks, M. Sees, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
10. *Modeling Biomass Fast Pyrolysis; Quantifying Effect of Intensification with Autothermal Operation*, with B. Caudle, R. Shukre, M.B. Gorensek, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018

11. *A New Local Composition Activity Coefficient Model for Mixed-Gas Adsorption Equilibria,* with H. Tun, H. Kaur, M. Sees, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
12. *Treating High Salinity Wastewater with Intensified Mechanical Vapor Compression-Membrane Distillation,* with M. Malmali, F. Hussain, R. Wickramasinghe, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
13. *Thermodynamic Modeling of CO_2 Absorption in Aqueous Amino Acid Salt Solutions with Symmetric Electrolyte NRTL Model,* with R. Shukre, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
14. *Combining Molecular Simulations and Theory for Predicting the Binary Interaction Parameters of the NRTL Model,* with A. Ravichandran, H. Tun, R. Khare, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
15. *Molecular Thermodynamic Model for Aqueous Na^+–K^+–Mg^{2+}–Ca^{2+}–Cl^-/SO_4^{2-} Quinary Electrolyte Systems,* with S. Tanveer, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
16. *Bridging Two-Liquid Theory with Molecular Simulations for Electrolytes: An Investigation of Aqueous NaCl Solution,* with S. H. Saravi, A. Ravichandran, R. Khare, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
17. *CFD Simulations for Gas Solubility Measurements with Gas-Liquid Segmented Flows,* with P. Vyawahare, M. Vaughn, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
18. *Thermodynamic Modeling of Electric Double Layer in Capacitive Deionization Cell Electrodes with Condensation Theory,* with Y. Yu, Y. Li, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
19. *Modeling the Ionic Transport in an Electrodialysis Cell: Investigating the Impacts of Non-Ideal Solution Behavior in the Cell,* with S. Honarparvar, D. Reible, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
20. *Refining the Nonrandom Two-Liquid Segment Activity Coefficient Model by Applying the Association Theory,* with Y. Hao, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
21. *Dynamics of Nucleation in 2D Monodisperse Oil-in-Water Emulsions,* with S. Abedi, S. Vanapalli, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
22. *Thermodynamic Modeling of Aqueous Multivalent Polyelectrolyte Systems with Polyelectrolyte NRTL Model*, with Y. Li, Y. Yu, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018
23. *Novel Steady State Process Modeling Methodology for Pressure Swing Adsorption,* M. Sees, T. Kirkes, T.-H. Kim, J. Scott, to be presented at 2018 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2018

24. *Thermodynamic Modeling of Polyelectrolyte Solutions with eNRTL Model*, with Y. Yu, presented at 20th Symposium on Thermophysical Properties, Boulder, CO, June 24-29, 2018
25. *Using Molecular Simulations for Predicting the Binary Interaction Parameters of the Non-Random Two-Liquid (NRTL) Model*, with A. Ravichandran, R. Khare, presented at 20th Symposium on Thermophysical Properties, Boulder, CO, June 24-29, 2018
26. *Dissociation Behavior of Ionic Liquids in Solvents: Thermodynamic Modeling and Molecular Dynamics Simulation,* with N. Hossain, R. Islam, R. Khare, presented at 20th Symposium on Thermophysical Properties, Boulder, CO, June 24-29, 2018
27. *Microfluidic Production of Size-Tunable n-Hexadecane-in-Water Emulsions: Effect of Droplet Size on Emulsion Destabilization due to Partial Coalescence*, with S. Abedi, S.A. Vanapalli, presented at 92nd ACS Colloid & Surface Science Symposium, State College, PA, June 10-13, 2018
28. *Thermodynamic Modeling of the LiCl + LiBr + $LiNO_3$ + LiI + H_2O System with Electrolyte NRTL* Model, with T. E. Kirkes, presented at 2018 AIChE Spring Meeting, Orlando, FL, April 22-26, 2018
29. *Application of Aggregation Thermodynamics and Molecular Characterization to Study Asphaltene Precipitation of Bituminous Crude Oils*, with Y. Hao, M.R. Islam, presented at 2018 AIChE Spring Meeting, Orlando, FL, April 22-26, 2018
30. *A Kinetic Analysis of the Shipp Synthesis of 2,2',4,4',6,6'-Hexanitrostibene from 2,4,6-Trinitrotoluene, with T.E. Kirkes, D. Ramirez, M. Haddix, presented at 2018 AIChE Spring Meeting, Orlando, FL, April 22-26, 2018*
31. *Thermodynamic Modeling for CO_2 Absorption in Aqueous Potassium Carbonate Solution with Electrolyte NRTL Model*, with H. Kaur, presented at 2018 AIChE Spring Meeting, Orlando, FL, April 22-26, 2018
32. *Pseudo-dynamic Aspen Plus Model of the Defense Waste Processing Facility*, with D.B. Henley, M.B. Gorensek, D.P. Lambert, presented at 2018 Waste Management Symposium, Phoenix, AZ, March 18-22, 2018 (rated "Superior Paper")

2017

33. *Thermodynamic Modeling of Ion Exchange Membranes with Electrolyte NRTL Model*, with Y. Yu, N. Yan, M. Galizia, B.D. Freeman, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
34. *Thermodynamic Modeling of Electrodes and Mobile Ions in Capacitive Deionization Cell Units with Electrolyte NRTL Model,* with Y. Yu, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
35. *Thermodynamic Modeling of Lithium Salt Systems with the Electrolyte NRTL Model*, with T. Kirkes, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
36. *CFD Simulation and Analysis of Gas-Liquid Segmented Flow with Mass Transfer in Microfluidic Devices: Case Study of CO2 Gas Solubility and Diffusivity Measurement in Aqueous NaCl Solution,* with P. Vyawahare, S. Abedi, M.W. Vaughn, F. Hussain, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017

37. *Can Molecular Simulations Predict the Binary Interaction Parameters of the Activity Coefficient Models?* with A. Ravichandran, R. Khare, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
38. *Prediction of Mean Ionic Activity Coefficient of NaCl-H_2O System at High Concentrations Using Molecular Dynamics Simulations,* with N. Hossain, A. Ravichandran, R. Khare, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
39. *Estimating NRTL-SAC Conceptual Segments of Molecules Using Sigma Profile,* with Y. Hao, M.R. Islam, M. Wang, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
40. *A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling, with Y. Hao, M.R. Islam, M. Wang, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017*
41. *A Modeling Methodology for Predicting Intensified CO_2 removal Efficiency with Rotating Packed Bed*, with C.-H. Hsiu, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
42. *Thermodynamic Model for Predicting Swelling of Poly(N-isopropyl acrylamide) Hydrogels in Solvent Mixtures,* with S. Tanveer, F. Hussain, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
43. *Comprehensive Thermodynamic Modeling of Mixed-Solvent Electrolyte Systems: An Investigation on the Quaternary System of $FeCl_2$-$FeCl_3$-HCl-H_2O,* with S.H. Saravi, presented at 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 29-Nov. 3, 2017
44. *From Molecular Simulations to Process Design − Predicting NRTL Binary Interaction Parameters from Molecular Simulations*, with A. Ravichandran and R. Khare, 2017 Global Grand Challenges Summit, Washington, DC, July 18-20, 2017
45. *Thermodynamic Modeling of Ion Absorption in Capacitive Deionization Cell Units with Electrolyte NRTL Model,* with Y. Yu and N. Hossain, International Conference on Capacitive Deionization, Electrosorption & Electrodialysis, KOFST, Seoul, Republic of Korea, July 3-6, 2017.
46. *Surfactant-Dependent Nucleation Kinetics in Monodisperse Hexadecane Emulsions*, with S. Abedi, S.A. Vanapalli, 91st ACS Colloid & Surface Science Symposium, The City College of New York, July 9-12, 2017
47. *Thermodynamic Modeling of HCl-H_2SO_4-H_2O Ternary System with Symmetric Electrolyte NRTL Model,* with H. Kaur*,* 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017
48. *Thermodynamic Modeling of Aqueous Copper(II) Nitrate – Chloride − Sulfate System with Electrolyte NRTL Model,* with B. Caudle and Y. Li*,* 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017
49. *Thermodynamic Modeling of Aqueous Nickel Nitrate-Nickel Chloride-Nickel Sulfate System with Electrolyte NRTL Model,* with Y. Li and B. Caudle, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017

50. *Thermodynamic Modeling of Ion Absorption in Capacitive Deionization Cell Units with Electrolyte NRTL Model,* with Y. Yu and N. Hossain, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.
51. *A Comprehensive Thermodynamic Model for Aqueous Lithium Chloride Binary System Using Electrolyte NRTL Model*, with T. Kirkes, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.
52. *Tracking Down Organic Acids and Sulfides from Petroleum Fluids: An Application of Real Molecule-Based Crude Assay Characterization and Segment-Based PC-SAFT*, with M. Wang, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.
53. *A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling,* with Y. Hao, M.R. Islam, M. Wang, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.
54. *Application of Aggregation Thermodynamics and Molecular Characterization to Study Asphaltene Precipitation of Bituminous Crude Oils,* with M.R. Islam, M. Wang, and Y. Hao, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.
55. *Process Intensification Toolkit for Mass and Heat Transfer in Rotating Packed Bed*, *with* C.H. Yu, 2017 AIChE Spring Meeting, San Antonio, TX, March 26-30, 2017.

2016

56. *TTU Chem-E-Car: Under Pressure,* with S. Vega, P. Chavez, C. Alvarez, A. Indah, J. Marston, and M. Vaughn, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
57. *Phase Behavior of Polymer Blends from Integral Equation Theory and Molecular Simulations*, with A. Ravichandran and R. Khare, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
58. *Application of Molecular Characterization to Bituminous Crude Oil to Study Asphaltene Precipitation*, with Md. Islam, Y. Hao, M. Wang, T. Kirkes, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
59. *Real-Component Based Molecular Characterization of Petroleum Fluids*, with M. Wang, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
60. *Application of Real-Component Based Molecular Characterization on Petroleum Refinery Simulation*, with M. Wang, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
61. *Comprehensive Thermodynamic Modeling of Complex Mixed-Solvent Electrolyte Systems: An Investigation on Water-Hydrogen Chloride-Methanol Ternary System*, with S.H. Saravi, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
62. *Thermodynamic Modeling of Produced Water with Electrolyte NRTL Model: Aqueous* Sr^{2+} - Na^{+} - SO_4^{2-} - Cl^{-} *Quaternary System*, with S. Honarparvar, D. Reible, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
63. *Thermodynamic Modeling of Polyelectrolyte Solutions with Electrolyte NRTL Model*, with Y. Yu, Y. Li, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.

64. *A Microfluidic Droplet Platform for Investigating Nucleation Kinetics of Hydrocarbons for Application to Wax Crystallization*, with S. Abedi, S. Vanapalli, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
65. *Determination of Enthalpy of Fusion of an Energetic Material, HMX, That Undergoes Simultaneous Fusion and* Decomposition, with S.K. Bhattacharia, B.L. Weeks, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
66. *Proper Consideration of Ionic Liquid Dissociation in Thermodynamic Modeling of Ionic Liquids and Mixtures*, with N. Hossain, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
67. *A Comprehensive Molecular Thermodynamic Model for Major Electrolytes in High Salinity Produced Water,* with S. Tanveer, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
68. *Modification of Staverman-Guggenheim Combinatorial Entropy Expression*, with Y. Hao, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
69. *Thermodynamic Modeling of the Hybrid Sulfur (HyS) Cycle for Hydrogen Production*, with H. Kaur, M. Wang, M.B. Gorensek, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
70. *Comparison between the OLI-MSE and eNRTL Models in Predicting Thermodynamic Properties of the $NaNO_3$-HNO_3-H_2O Ternary System*, with M. Wang, M.B. Gorensek, 2016 AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
71. *Microfluidic Study of CO_2 Dissolution and Solubility in Aqueous Electrolyte Solutions*, with S. Abedi, S.A. Vanapalli, 90th ACS Colloid & Surface Science Symposium, Cambridge, MA, June 5-8, 2016
72. *Development of a Comprehensive Molecular Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions,* with T. Sheik and H. Zhou, Properties and Phase Equilibria for Product and Process Design 2016 Conference, Porto, Portugal, May 22-26, 2016
73. *Predicting Asphaltene Precipitation in Petroleum Fluids via NRTL-SAC*, with Md Islam, Properties and Phase Equilibria for Product and Process Design 2016 Conference, Porto, Portugal, May 22-26, 2016
74. *Thermodynamic Modeling of HNO_3-H_2SO_4-H_2O Ternary System with Symmetric Electrolyte NRTL Model*, with M. Wang, H. Kaur, 2016 AIChE Spring Meeting, Houston, TX, April 10-14, 2016
75. *Explaining the Paradox of Asphaltene Precipitation with n-Alkanes*, with Md Islam, Y. Hao, M. Wang, T. Kirkes, 2016 AIChE Spring Meeting, Houston, TX, April 10-14, 2016
76. *A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling*, with Y. Hao, 2016 AIChE Spring Meeting, Houston, TX, April 10-14, 2016
77. *Thermodynamic Modeling of CO_2 Solubility in Aqueous Solutions of NaCl, KCl, $CaCl_2$, $MgCl_2$ and Their Mixed Salts Using eNRTL Model*, with S. Adebi, 2016 AIChE Spring Meeting, Houston, TX, April 10-14, 2016

78. *Thermodynamic Modeling of Aqueous Lithium Sulfate and Its Solubility in the Presence of Na^+, K^+ and Mg^{2+} Sulfates*, with S. Adebi, 2016 AIChE Spring Meeting, Houston, TX, April 10-14, 2016
79. *Effect of Chain Length and Chain Conformation on χ Parameter for Polyolefin Blends: A Molecular Dynamics Study,* with A. Ravichandran and R. Khare, APS March Meeting 2016, Baltimore, MD, March 14-18, 2016

2015

80. *Modeling of Hydrogen-Bromine Flow Battery System: Thermodynamics Perspective*, with Y. Yu, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
81. *Molecular Thermodynamic Modeling of a Two-Step Asphaltene Precipitation Process,* with M. Wang, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
82. *Thermodynamic Modeling of Water-Hydrogen Chloride-Methanol System,* with S.H. Saravi, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
83. *Thermodynamic Modeling of Binary, Ternary and Quaternary Aqueous Solutions Containing Ba^{2+}, Na^+, Cl^-, and SO_4^{2-} By eNRTL Model,* with S. Honarparvar and D. Reible, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
84. *Determination of the Chi Parameter for Polymer Blends from Molecular Simulations*, with A. Ravichandran and R. Khare, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
85. *Employing Modeling Techniques to Predict the Solubility of Hesperetin in Binary Solvent Systems*, with M. Hansen, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
86. *Microfluidic Study of CO2 Solubility in Aqueous Single and Mixed-Electrolyte Solutions*, with S. Abedi, S. Vanapalli, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
87. *A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling*, with Y. Hao, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
88. *Prediction of Asphaltenes Precipitation upon Blending of Petroleum Fluids*, with M.R. Islam, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
89. *Comprehensive Thermodynamic Model for Aqueous Nitric Acid and Sodium Nitrate Solution with Electrolyte NRTL Equation*, with M.B. Gorensek, D.P. Lambert, and M. Wang, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
90. *A Predictive Viscosity Expression for Aqueous Electrolyte Solutions*, with M. Kovalski, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
91. *Thermodynamic Solubility Modeling of 2,4,6-Trinitrotoluene (TNT)*, with N. Hossain and S.K. Bhattacharia, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015
92. *Temperature Dependence of Interaction Parameters of Electrolyte NRTL Model,* with N. Hossain, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015

93. *Thermodynamic Model for Aqueous Na^{+}–K^{+}– Mg^{2+}–SO_4^{2-} Quaternary System*, with S.K. Bhattacharia and N. Hossain, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015

94. *Thermodynamic Modeling of Quaternary Aqueous Mg^{2+}, Na^{+}, K^{+}, Cl^{-} System,* with S. Tanveer, 2015 AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015

95. *Thermodynamic Solubility Modeling of Organic Energetic Materials*, with S.K. Bhattacharia, N. Hossain and B.L. Weeks, Inaugural Meeting of the National Energetic Materials Consortium, Lubbock, TX, October 13, 2015

96. *χ Parameter Estimation for Polymer Blends from Molecular Simulations – Integral Equation Theory Based Approach,* with A. Ravichandran and R. Khare, LAMMPS Users' Workshop and Symposium, Albuquerque, NM, August 5-7, 2015

97. *Temperature Dependency of Interaction Parameters of Electrolyte NRTL Model*, with N. Hossain, 19th Symposium on Thermophysical Properties, Boulder, CO, June 21-26, 2015

98. *Prediction of Asphaltene Solubility in Organic Solvents via NRTL-SAC and COSMO-SAC*, with M. Wang, Y. Hao, and M.R. Islam, 2015 AIChE Spring Meeting, Austin, TX, April 26-30, 2015

99. *Thermodynamic Modeling of Aqueous Ca^{+2}, Na^{+}, K^{+}, Cl^{-} Quaternary System*, with S. Tanveer, 2015 AIChE Spring Meeting, Austin, TX, April 26-30, 2015

100. *Thermodynamic Modeling of Br_2-HBr-H_2O Ternary System with eNRTL Model*, with Y. Yu, 2015 AIChE Spring Meeting, Austin, TX, April 26-30, 2015

101. *Estimation of χ Parameter from Molecular Simulations*, with A. Ravichandran and R. Khare, 2015 APS Meeting, San Antonio, TX, March 2-6, 2015

2014

102. *Sigma Profile Generation with Conceptual Segment Approach*, with M.R. Islam, 2014 AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014

103. *Development of Saline Water Thermodynamic Model for Hydraulic Fracturing*, with S.H. Saravi, 2014 AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014

104. *Expression for Aqueous Multicomponent Electrolyte Viscosity Based on Andrade Equation*, with M. Kovalski, 2014 AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014

105. *Smart Manufacturing: Replacing Analytical Sample Control with Model Predictive Control*, with M.B. Gorensek, D.P. Lambert, and T.B. Edwards, Savannah River National Laboratory, Aiken, SC, October 15, 2014

106. *Thermodynamic Modeling of Solutions of Sodium Nitrate and Nitric Acid*, with M. Wang, M.B. Gorensek, D.P. Lambert, 42nd Annual Conference of North American Thermal Analysis Society, Santa Fe, NM, September 14-17, 2014

107. *Modeling Concentration and Temperature Dependence of Thermodynamic Properties of Aqueous Electrolyte Solutions: Investigation of K^{+}-Cl^{-}-SO_4^{-2}-H_2O System*, with S.K.

Bhattacharia and N. Hossain, 42nd Annual Conference of North American Thermal Analysis Society, Santa Fe, NM, September 14-17, 2014

108. Ion-Size Based Andrade Expression for Brine Solution Viscosity, with M. Kovalski, Fracturing Impacts and Technologies Conference, Lubbock, Texas, September 4-5, 2014

109. Correlations for Density of Aqueous Electrolyte Solutions, with N. Nguyen, Fracturing Impacts and Technologies Conference, Lubbock, Texas, September 4-5, 2014

110. Development of a Comprehensive Thermodynamic Model for Scale Formation of Saline Water in Hydraulic Fracturing Conditions, with S. Honarparvar, Fracturing Impacts and Technologies Conference, Lubbock, Texas, September 4-5, 2014

111. Direct Solar Hybrid Sulfur Water-Splitting Process for Continuous Centralized Hydrogen Production, with B.Wong, H. Colón-Mercado, D. Ginosar, M. Gorensek, J.R. Monnier, M. Roeb, W. Summers, D. Thomey, J.W. Weidner, 20th World Hydrogen Energy Conference, Gwangju, S.Korea, June 15-20, 2014

2013

112. A Practical Molecular Thermodynamic Model for Asphaltene Aggregation, 2013 AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013

113. Crude Evaluation for Refinery Planning Using a Molecular-Based Assay Characterization, 2013 AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013

114. Molecule-Based Assay Characterization Methodology for Correlation and Prediction of Properties for Crude Oil and Petroleum Fraction, Properties and Phase Equilibria for Product and Process Design 2013 Conference, Iguazu Falls, Argentina – Brazil, May 26-30, 2013

115. Molecular Based Assays for Practical Correlation and Prediction of Crude Oil and Petroleum Fraction Properties, 2013 AIChE Spring Meeting and 9th Global Congress on Process Safety, San Antonio, Texas, April 28-May 2, 2013

2012

116. Rate-Based Modeling of CO_2 Capture Pilot Plant with Aqueous Monoethanolamine Solution, 11th International Conference on Greenhouse Gas Control Technologies (GHGT-11), Kyoto, Japan, November 18-22, 2012

117. Rate-Based Modeling of CO_2 Absorption and Desorption into Aqueous Monoethanolamine Solutions, AIChE Annual Meeting, Pittsburgh, Pennsylvania, October 28-November 2, 2012

2011

118. AspenTech – Leading the Understanding of Modeling CO_2 Capture, AspenTech Global Conference, Washington D.C., May 23-25, 2011

2010

119. Opportunities, Challenges and Advances in Process Simulation and Applied Thermodynamics, AIChE Annual Meeting, Salt Lake City, Utah, November 7-12, 2010

120. Extension of COSMO-SAC Solvation Model for Electrolytes, with S. Wang and Y. Song, AIChE Annual Meeting, Salt Lake City, Utah, November 7-12, 2010

121. Development of a Segment-Based DEPG Physical Solvent Model for CO_2 Capture Processes, 35th International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference"), Clearwater, Florida, June 6-10, 2010

122. Development of an Aspen Plus Model for Scaling Prediction, with C. Yan, Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

123. Electrolyte NRTL Model for Thermodynamic Representation of CO_2 Absorption in Aqueous Monoethanolamine and 2-Amino-2-methyl-1-propanol Solutions, with Y. Zhang, Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

124. Development of a DEPG-Based CO_2 Capture Process Model, with L. Zong, Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

125. Novel Approach for Estimating Thermophysical Properties of Lignocellulosic Biomass for Process Modeling and Simulation, with X.-F. Chang, Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

126. Thermodynamic Modeling of the Sulfuric Acid-Water-Sulfur Trioxide System with Symmetric Electrolyte NRTL Model, with H.-L. Que, Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

2009

127. Thermodynamic Modeling of the Sulfuric Acid-Water-Sulfur Trioxide System with the Symmetric Electrolyte NRTL Model, AIChE Annual Meeting, Nashville, TN., November 8-13, 2009

128. Modeling and Simulation in Support of Quality by Design, AIChE Annual Meeting, Nashville, TN., November 8-13, 2009

129. Novel Approach for Estimating Thermophysical Properties of Fats and Vegetable Oils for Biodiesel Production Processes, with R. Hockley, L. Zong, and S. Ramanathan, ACHEMA 2009, Frankfurt am Main, Germany, May 11-15, 2009

130. What's New: Aspen Solubility Modeler, Aspen Worldwide User Conference, Houston, Texas, May 4-7, 2009

2008

131. Formulation and Behavior of a Symmetric Electrolyte NRTL-SAC Model for Excess Gibbs Energy of Electrolyte Systems, with Y. Song and G.M. Bollas, AIChE Annual Meeting, Philadelphia, Pennsylvania, November 16-21, 2008

132. Refined Electrolyte-NRTL Model: Inclusion of Hydration for the Detailed Description of Electrolyte Solutions. Part I. Single Electrolytes up to Moderate Concentrations, Single Salts up to the Solubility Limit, with G.M. Bollas and P.I. Barton, AIChE Annual Meeting, Philadelphia, Pennsylvania, November 16-21, 2008

133. *Model Based Solvent Selection with NRTL-SAC Including Use of Chromatographic Retention Times as Model Input,* with A.J. Marchut and O. Lyngberg, AIChE Annual Meeting, Philadelphia, Pennsylvania, November 16-21, 2008

134. *A Rate-Based Process Modeling Study of CO_2 Capture with Aqueous Amine Solutions Using aspenONE process Engineering*, 33rd International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference"), Clearwater, Florida, June 1-5, 2008

135. *AspenTech Research Initiatives*, AspenTech China User Group Meeting, Hangzhou, China, May 27-28, 2008

136. *AspenTech R&D Initiatives in 2006.5 and Future Release,* AspenTech Japan User Group Meeting, Tokyo, Japan, May 20-21, 2008

137. *Rate-Based CO_2 Capture Solvent Packages in aspenONE 2006.5*, AspenTech Japan User Group Meeting, Tokyo, Japan, May 20-21, 2008

138. *A Rate-Based Process Modeling Study of CO_2 Capture with Aqueous MEA Solution*, with Rob Hockley, IChemE's Fluid Separations Subject Group Technical Meeting on Capture of CO2 from Combustion Processes, University College London, London, UK, April 18, 2008

2007

139. *A Rate-Based Process Modeling Study of CO_2 Capture with Aqueous MEA Solution,* with Davy Zuo, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007

140. *The Significance of Mixing Rules, Hydration and Complex Formation in the electrolyte NRTL Model*, with G.M. Bollas and P.I. Barton, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007

141. *Solubility Modeling from High Throughput Solvent Screening*, with Jose E. Tabora, paper AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007

142. *A Practical Molecular Thermodynamic Model for Pharmaceutical Industry*, 11th International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, May 20-25, 2007

143. *New Technologies for Product-on-Demand Design,* with M. Frenkel, S. Watanasiri, R.D. Chirico, V. Diky and C. Muzny, 11th International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, May 20-25, 2007

144. *Solubility in Process and Product Development of Pharmaceuticals,* with H.-H. Tung et al., AspenTech NALA Pharmaceutical Seminar on aspenONE for Process Development, East Princeton, NJ, May 16, 2007

145. *Models, Tools and Best Practices in Solubility Modeling*, AspenTech NALA Pharmaceutical Seminar on aspenONE for Process Development, East Princeton, NJ, May 16, 2007

2006

146. *RateSep – A New and Innovative Rate-Based Distillation Model for Amine Gas Treating Processes*, AIChE Annual Meeting, San Francisco, CA, November 12-17, 2006

147. *Modeling Pharmaceutical Salt Solubility in Mixed Solvents with eNRTL-SAC*, with H.-H. Tung, AIChE Annual Meeting, San Francisco, CA, November 12-17, 2006

148. *Modeling Drug Molecule Solubility with the NRTL Segment Activity Coefficient Model*, with Prashant B. Kokitkar, 14th Larson Workshop of Association of Crystallization Technology, Princeton, NJ, October 8-11, 2006

149. *Correlation and Prediction of Drug Molecule Solubility with the NRTL-SAC Model*, with Peter A. Crafts, 16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering, Garmisch-Partenkirchen, Germany, July 9-14, 2006

150. *Predicting Pharmaceutical Solubility with Aspen's NRTL-SAC Model*, with P. Crafts, D. Horner, M. Jones, J. Koningen, I. McConvery, AstraZeneca PE Conference 2006, Macclesfield, U.K., June 11, 2006

151. *Product Direction for AspenONE Process Modeling – Chemicals*, AspenTech China User Group Meeting, Shanghai, China. May 25-26, 2006

152. *RateSep – A New and Innovative Rate-Based Distillation Model for Amine Acid Gas Treating* Processes, with S. Oba, T. Suzuki, S. Anavi, H. Chen, J.-J. Peng, and H.-L. Li, 4th International Symposium on Molecular Thermodynamics and Molecular Simulation, Chiba, Japan, May 23-25, 2006

2005

153. *Solubility Prediction of Pharmaceuticals in Pure and Mixed Solvents with NRTL-SAC,* with Peter A. Crafts, Aspen Engineering User Group Meeting, Amsterdam, The Netherlands, November 7-8, 2005

154. *Estimating Solubility of Organic Salts with eNRTL-SAC Model*, with Y. Song, AIChE Annual Meeting, Cincinnati, OH, October 30 - November 1, 2005

155. *VT-2005 Sigma-Profile Database: An Open Literature Database of Sigma Profiles for 1055 Organic Molecules,* with E. Mullins, Y.A. Liu, R. Oldland, S. Wang, S.I. Sandler, M. Zwolak, and K.C. Seavey, Aspen Engineering User Group Meeting, Houston, TX, October 24-25, 2005

156. *Prediction of Pharmaceuticals Solubility via NRTL-SAC and COSMO-SAC,* with Hsien-Hsin Tung, Nara Variankaval, Jose Tabora, and Daniel Bakken, 16th International Symposium on Industrial Crystallization, Dresden, Germany, September 11-14, 2005

157. *Solubility Modeling with the Non-Random Two-Liquid* S*egment Activity Coefficient Model,* 2nd Annual CHI Predictive ADME Conference, San Diego, CA, January 10-11, 2005

2004

158. *A Practical Phase Equilibrium Model for Solvent Selection in Pharmaceutical Industry – Organic Electrolytes*, with Y. Song, AIChE Annual Meeting, Austin, TX, November 7-12, 2004

159. *Solubility Modeling and Design of Crystallization Processes*, with J.E. Tabora, H.-H. Tung, D. Bakken, and Yuhua Song, ASPENWOLRD 04, Orlando, Florida, October 10-15, 2004

160. Viscosity Model for Mixtures Containing Polymers, with Lawrence T. Novak and Yuhua Song, ASPENWOLRD 04, Orlando, Florida, October 10-15, 2004

161. Polymer Thermodynamics for Process Modeling, with Y. Song, paper AIChE National Meeting, New Orleans, LA, April 25-29, 2004

2003

162. AspenTech's Engineering Solutions for Chemicals and Polymers, AspenTech China 2003 Information Technology Forum & User Group Meeting, Beijing, China, December 3-4, 2003

163. A Practical Phase Equilibrium Model for Solvent Selection in Pharmaceutical Industry, AIChE Annual Meeting, San Francisco, CA, November 16-21, 2003

164. Polymers Plus Development Directions, with D.A. Tremblay, AspenTech User Group Meeting, New Orleans, LA, October 5-8, 2003, and Paris, France, October 19-22, 2003

165. A Generalized Electrolyte NRTL Model for Mean Ionic Activity Coefficients of Mixed-Solvent Electrolyte Systems, AspenTech User Group Meeting, Paris, France, October 19-22, 2003

166. A New POLYMIX-Based Algorithm to Solve Complex Phase Behavior of Polymer Systems, with R.D. Swindoll, P.K. Jog, S. Lingard, and Y. Song, AspenTech User Group Meeting, New Orleans, LA, October 5-8, 2003, and Paris, France, October 19-22, 2003

167. Solubility Modeling in Pharmaceutical Process Design, with D. Bakken, J.E. Tabora, H.-H. Tung, O. Davidson, M. Thien, C. Rentsch, and Y. Song, AspenTech User Group Meeting, New Orleans, LA, October 5-8, 2003, and Paris, France, October 19-22, 2003

168. Phase Equilibrium Predictions and Applications with COSMO Solvation Models, with S. Oba, P.M. Mathias, and Y. Song, 3rd International Symposium on Molecular Thermodynamics and Molecular Simulation, Sendai, Japan, May 27-30, 2003

169. Facilitating Property Calculation within the Product and Process Lifecycle, with V. De Leeuw, Laboratory of Thermodynamics and Phase Equilibrium, Center of Energetics, Ecole de Mines, March 28, 2003

2002

170. Improvements of Phase Equilibrium Predictions for Hydrogen-Bonding Systems from a New Energy Expression with COSMO Solvation Models, with P. M. Mathias, S. I. Sandler, Y. Song, and S.-T. Lin, AIChE Annual Meeting, Indianapolis, IN., November 3-8, 2002

171. Industrial Perspectives on Polymer Process Modeling: Accomplishments, Deficiencies, and Opportunities, with R. Swindoll and K.-D. Hungenberg, ASPENWORLD 02, Washington D.C., October 27-November 1, 2002

172. Melt Index Prediction Using the Polymer Molecular Weight Distribution, with K.C. Seavey, N.P. Khare, Y.A. Liu and T.N. Williams, ASPENWORLD 02, Washington, D.C., October 27-November 1, 2002

173. Polymers Plus – A Status Report, ASPENWORLD 02, Washington, D.C., October 27-November 1, 2002

174. Applied Thermodynamics in Industrial Applications – Vision on Technology and Economic Impact on Process Industry, with S. Oba, Y. Kumagae and P.M. Mathias, 6th International Symposium on Separation Technology between Japan and Korea, October 2002

175. Melt Index Prediction Using the Polymer Molecular Weight Distribution, with K.C. Seavey, N.P. Khare, Y.A. Liu and T.N. Williams, AIChE Spring Meeting, New Orleans, LA, March 10-14, 2002

176. Simulation of Electrolyte Processes - Status and Challenges, with P. M. Mathias, AIChE Spring Meeting, New Orleans, LA, March 10-14, 2002

2001

177. A Representation of the Thermodynamic Properties of Sulfuric Acid and Oleum, with P.M. Mathias, B.-S. Zou, D.L. Randolph III and F.J. Doering, AIChE Annual Meeting, Reno, NV, November 4-9, 2001

178. Thermodynamic Model for the HI-I_2-H_2O System, with P.M. Mathias, L.C. Brown and D. Ramrus, AIChE Annual Meeting, Reno, NV, November 4-9, 2001

179. Design of Polymer Processes using the Coupling of Commercial Simulation Packages Polymers Plus® and PREDICI®, 7th Polymer Reaction Engineering Workshop, Hamburg, Germany, October 8-10, 2001

180. Application of the Electrolyte-Polymer NRTL Model to Liquid-Liquid Equilibrium of Aqueous Solutions Containing Polymer and Salt, with C.P. Bokis and P.M. Mathias, AIChE Spring National Meeting, Houston, TX, April 22-26, 2001

2000

181. A Segment-Based Excess Gibbs Energy Model for Aqueous Organic Electrolyte Systems, with C.P. Bokis and P.M. Mathias, AIChE Annual Meeting, Los Angeles, CA, November 13-17, 2000

182. Modeling Polyethylene Fractionation Using the Statistical Associating Fluid Theory, with C.P. Bokis and E. Cheluget, J. Fisher and L. Wardhaugh, Third Joint China/USA Chemical Engineering Conference, Beijing, China, September 25-28, 2000

183. Modeling the Complex Chemical Reactions and Mass Transfer in a Phosphoric Acid Reactor, with P.M. Mathias and M. Walters, Third Joint China/USA Chemical Engineering Conference, Beijing, China, September 25-28, 2000

184. Development and Application of HDPE Reaction Simulation Model, Aspen World China, Beijing, China, July 13-14, 2000

185. Use AspenTech Polymer Modeling Solution to Capture, Communicate and Apply Process Fundamentals in R&D, Process Engineering, and Training Operators, ASPENWORLD 2000, Orlando, Florida, February 6-11, 2000

1999

186. Unification of Hydration and Dissociation Chemistries with the Electrolyte NRTL Model, with P.M. Mathias and H. Orbey, AIChE Annual Meeting, Dallas, TX, Oct 31-Nov 5, 1999

187. Physical Properties and Phase Equilibria in Polymer Process Simulation, with C.P. Bokis and H. Orbey, AIChE National Meeting, Houston, TX, March 14-18, 1999

1997

188. Opportunities and Challenges for Simulation in the Inorganic-Chemicals, Metals and Mining Industries, with P.M. Mathias, P. Talley and M. Mendez, ASPENWORLD 97, Boston, MA, October 13-15, 1997

189. A Practical Emulsion Copolymerization Model - II. Homogeneous Nucleation, with S.R. Ponnuswamy and F. Bettenwort, ASPENWORLD 97, Boston, MA, October 13-15, 1997

1996

190. Design, Control, and Optimization of Polymerization Processes, with T. Mock, Chemputers IV Conference, Houston, Texas, March 1996

191. A Phase-Equilibrium Model for Semi-Crystalline Polymers, with D. Embry, AIChE Spring National Meeting, New Orleans, February 25-29, 1996

1995

192. An Industrial Perspective in Modeling Polymer Reactors and Processes, with S.Ramanathan, D.A. Tremblay, K. Ravindranath, M. Osias, and T. Mock, Seminar on Process Modeling for Operator Training, Simulation and Optimization, Antweep, Belgium, Oct 12, 1995

1994

193. AspenTech Polymers Technology Program, ASPENWORLD 94, Boston, MA. November 6-9, 1994

194. BioProcess Simulation: Meeting the Challenges for Today's Pharmaceutical and Biotechnology Industries, with Y. Zhu and J.G. Stramondo, AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994

195. Computer Modeling of Chemical Processes with Electrolytes, Symposium on Basic Chemistry for Industrial Applications, ACS National Meeting, Washington, D.C., August 21-25, 1994

1992

196. Thermodynamic Analysis in Protein Aggregation and Protein Refolding, 7th Annual BPEC Symposium on Protein Processing & Protein Interactions, MIT, Cambridge, Mass., November 23-24, 1992

197. Simulation of Polymer Manufacturing Plants, with S. Ramanathan, M. Barrera, M. Osias, D.A. Tremblay, and G. Ko, 4th International Workshop on Polymer Reaction Engineering, Berlin, Germany, October 12-14, 1992

198. Application of Simulation to Agrichemical Processes, with D. Denholm, Pao-Chen Wu, AIChE Annual Meeting, Miami Beach, FL, 1992

199. A Segment-Based Local Composition Model for the Gibbs Energy of Polymer Solutions, 6th International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, Cortina d'Ampezzo, Italy, July 19-22, 1992

200. Process Simulation in Polymer Manufacturing, with G.H. Ko, M. Osias, D.A. Tremblay, and M.D. Barrera, European Symposium on Computer Aided Process Engineering (ESCAPE-1), Elsinore, Denmark, May 24-28, 1992

1991

201. Molecular Thermodynamic Modeling of Polypeptide Chain Folding, with L.B. Evans and Y. Zhu, ASPENWORLD 91, Boston, MA, November 3-6, 1991

202. Simulation of MSW Incineration in a Water-Walled Rotary Combustor, with W.-C. Yang, N.H. Ulerich, S.V. Dighe, and I.H. Farag, ASPENWORLD 91, Boston, MA, November 3-6, 1991

203. Modeling of a Partition-Transmutation-Disposal System with ASPEN PLUS, with B.J. Knutson, L.G. Niccoli, G. Jansen, and I.H. Farag, ASPENWORLD 91, Boston, MA, November 3-6, 1991

204. Simulation of Polymer Processes with Aspen Plus™, with G.H. Ko, M. Barrera, D.A. Tremblay, and M. Oasia, ACHEMA 91, Frankfurt am Main, Germany, June 9-15, 1991

205. Addressing Industrial Waste Treatment Problems by Simulation, with I.H. Farag and D.L. Denholm, ACHEMA 91, Frankfurt am Main, Germany, June 9-15, 1991

206. Modeling of the CURE Partition-Transmutation System with the Aspen Plus Flowsheet Simulator, with L.G. Niccoli, G. Jansen, Jr., and I.H. Farag, Emerging Technologies for Waste Management, 1991 Industrial & Engineering Chemistry Division Special Symposium, American Chemical Society, Atlanta, GA, Oct 1-3, 1991

207. Process Modeling of Food Processing Systems, with M.-W. Hsieh, Conference of Food Engineering (CoFE'91), Chicago, IL., March 11-13, 1991

208. Simulation of Food Processes Using Aspen Plus or BPS, with D. Denholm, I. Gosling, and P. Chan, Conference of Food Engineering (CoFE'91), Chicago, IL., March 11-13, 1991

1990

209. Modeling of the CURE Partition-Transmutation System with the Aspen Plus Flowsheet Simulator, with L.G. Niccoli, G. Jansen, Jr., and I.H. Farag, Winter Meeting of the American Nuclear Society, Washington, D.C., November 11-16, 1990

210. Improving Pollution Prevention Process Design by Simulation, with I.H. Farag, P.-C. Wu, and J. Rosen, AIChE Summer National Meeting, San Diego, CA, August 19-22, 1990

211. Application of Aspen Plus in Simulation of High Pressure Tubular Polyethylene Reactor, with G.H. Ko and S. Anavi, AIChE National Meeting, Orlando, FL., March 1990

212. A Segment-Based Molecular Thermodynamic Model for Phase Behavior of Biomolecules, with Y. Zhu and L.B. Evans, AIChE National Meeting, Orlando, FL., March 1990

1989

213. *A Model of Vapor-Liquid Equilibria for Aqueous Gas-Alkanolamine Systems. II. Representation of H_2S and CO_2 Solubility in MDEA and CO_2 Solubility in Aqueous MDEA and MEA or DEA,* with D. Austgen and G.T. Rochelle, AIChE Spring Meeting, Houston, TX, 1989

214. *Applications Modeling Project Execution,* AspenTech Japan User Group Meeting, Kyoto, Japan, 1989

215. *Application of Aspen Plus in the Pulp & Paper Industry,* with D. Denholm, AIChE Annual Meeting, November 5-10, 1989

1988

216. *Ionic Activity Coefficients of Mixed-Solvent Electrolyte Systems,* ASPENWORD 88, Amsterdam, Netherlands, November 13-16, 1988

217. *Phase Partitions of Biomolecules – Solubilities of Amino Acids,* with L.B. Evans and Y. Zhu, ASPENWORD 88, Amsterdam, Netherlands, November 13-16, 1988

218. *A Physical Property Model for Caustic Evaporator,* with J. Gibson, D. Phipps and P. Collier, ASPENWORD 88, Amsterdam, Netherlands, November 13-16, 1988

219. *Model of Vapor-Liquid Equilibria for Aqueous Gas Alkanolamine Systems Using the Electrolyte NRTL Model,* with D.M. Austgen, G.T. Rochelle, and X. Peng, AIChE Spring Meeting, New Orleans, LA, 1988

220. *Role of Computerized Modeling and Simulation in the Development of Life Support System Technology,* with M. Modell, P. Evanich, S. Anavi, and J. Mai, 27th Meeting of the Committee on Space Research, Espoo, Finland, July 18-29, 1988

221. *A Representation of Thermodynamic Properties of Aqueous Sulfuric Acid,* with S.M. Goldfarb, 10th Symposium on Thermophysical Properties, National Bureau of Standards, Gaithersburg, Maryland, April 1988

222. *A Representation of Thermodynamic Properties of Aqueous Sulfuric Acid,* with R.A. Trevino-Lozano and S.M. Goldfarb, Modeling and Simulation of Metallurgical & Chemical Processes, Mons, Belgium, May 9-10, 1988

223. *Process Simulation of Polymerization Processes,* with T.L. Mock, D.L. Phipps, Jr., and R.A. Greenberg, AIChE Spring Meeting, New Orleans, LA, March 6-8, 1988

1987

224. *An Algorithm for Solving Simultaneous Phase and Chemical Equilibria of Electrolyte Systems,* with Jin-Qing Yang, AIChE Annual Meeting, New York, NY, November 15-20, 1987

225. *Computer Simulation in Design of Hazardous Waste Treatment Processes,* with E.D. Treworgy and D.P. Ostrye, Hazardous Materials Management Technical Conference, Chattanooga, TN, June 8-12, 1987

226. *Simulation of Electrolyte Systems with Aspen Plus,* with H.I. Britt and J.F. Boston, International Conference on Thermodynamics of Aqueous Systems with Industrial Applications, Airlie House, Warrenton, VA, May 10-14, 1987

1986

227. Process Simulation of Metallurgical Processes, with H.J. Herzog, J.D. Lenoir and L. Crabs, Benelux Process Control in Metallurgy Symposium, Brussels, Belgium, May 1986

1985

228. Representation of Solid-Liquid Equilibrium of Aqueous Electrolytes with the Electrolyte NRTL Model, International Meeting on Phase Equilibrium Data, Paris, France, September 5-13, 1985

229. Computer Simulation of an Existing Ammonia Plant, with S.C. Moore and T.M. Piper, 1985 AIChE Ammonia Safety Symposium, Seattle, August 25-28, 1985

1984

230. Thermodynamic Representation of Phase Equilibria in Multiple-Solvent Electrolyte Systems, with B. Mock and L.B. Evans, AIChE Annual Meeting, San Francisco, CA, November 25-30, 1984

231. A Local Composition Model for the Excess Gibbs Energy of Multicomponent Aqueous Electrolyte Systems, with L.B. Evans, AIChE Annual Meeting, San Francisco, CA, November 25-30, 1984

232. Computer-Aided Engineering of Electrolyte Systems, with L.B. Evans, AIChE Annual Meeting, San Francisco, CA, November 25-30, 1984

233. Process Simulation of Electrolyte Systems, with H.I. Britt and J.F. Boston, 1984 Summer Computer Simulation Conference, Boston, MA, July 23-25, 1984

234. Phase Equilibria in Multiple-Solvent Electrolyte Systems: A New Thermodynamic Model, with B. Mock and L.B. Evans, 1984 Summer Computer Simulation Conference, Boston, MA, July 23-25, 1984

235. Bayer Process Simulation by ASPEN, with J.F. Boston, T.J. Galloway, K.Y. Lee and B. Mock, AIChE National Meeting, Anaheim, CA, April 1984

1983

236. New Capabilities in ASPEN PLUS, with J.F. Boston, H.I. Britt, L.B. Evans and P.W. Gallier, Systems Simulation Symposium of Fossil Fuel Conversion Processes, Morgantown VA, December 1983

237. Thermodynamic Property Evaluation in Computer-Based Flowsheet Simulation for Aqueous Electrolyte Systems, with H.I. Britt, J.F. Boston and W.M. Clarke, AIChE National Meeting, Denver, CO, August 28-31, 1983

238. Bayer Process Simulation by ASPEN, with J.F. Boston, T.J. Galloway, K.Y. Lee and B. Mock, AIME Meeting, Atlanta, GA, March 1983

1981

239. Modeling of an Oil-Shale Fluidized-Bed Retorting Process Using ASPEN, with L.B. Evans, J. Floess, L. Fong and J.P. Longwell, AIChE Meeting, Detroit, MI, August 1981

240. ASPEN Electrolyte Simulation Capabilities, with J.F. Boston, H.I. Britt, and L.B. Evans, AIChE National Meeting, Houston, TX, April 1981

1979

241. Two New Activity Coefficient Models for the Vapor-Liquid Equilibrium of Electrolyte Systems, with H.I. Britt, J.F. Boston and L.B. Evans, Conference on the Thermodynamics of Aqueous Systems with Industrial Applications, Airlie House, Warrenton, VA, October 22-25, 1979