Chau-Chyun Chen

Jack Maddox Distinguished Chair in Engineering
Department of Chemical Engineering
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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

July 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

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
Chinese American Chemical Society
U.S. National Academy of Engineering

Professional Activities and Services

- 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
- Board Member, Advisory Board of Science and Technology for the National Institute of Clean-and-Low-Carbon Energy, Shenhua Group, China, 2009 – present
- Board Member (Industrial Trustee), the Computer Aids for Chemical Engineering Education (CACHE) Corporation (Not-for-Profit), 2003 – present
- Editorial Board Member of *Fluid Phase Equilibria*, 2001 – present
- 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"

RESEARCH ACTIVITIES

Summary of Research Productivity (as of 7/27/2013)

- Web of Science Citations: 2564 total citations, 67 articles with citation data, 38.3 citations per article, h-index of 24
- Refereed Journal Articles: 69 published
- Other Journal Articles: 14 published
- Refereed Book Chapters: 7 published
- Refereed Proceedings: 13 published
- Invited Lectures: 34
- Conference Presentations: 128
- Patents Granted: 13
- Patents Pending: 9
- Research Interests: 1) Molecular thermodynamics, Thermophysical properties and fluid phase equilibria, Process modeling and simulation; 2) Petroleum crude characterization, Hydraulic fracturing & flow-back fluids; 3) CO_2 capture systems, Energy storage systems, 4) Pharmaceutical solubility modeling

Patents and Pending Patents

1. C.-C. Chen, H. Que, "Method of Characterizing Chemical Composition of Crude Oil for Petroleum Processing," U.S. Patent Application No.: 2013/0185044, July 18, 2013.
2. C.-C. Chen, H. Que, "Method of Characterizing Chemical Composition of Crude Oil for Petroleum Processing," PCT International Application No.: PCT/US13/21294, January 11, 2013.
3. 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. 8,370,076**, February 5, 2013.
4. C.-C. Chen, Y. Song, "Methods of Modeling Physical Properties of Chemical Mixtures and Articles of Use," **U.S. Patent No. 8,346,525 B2**, January 1, 2013.
5. H. Xiang, S. Anavi, C.-C. Chen, "Systems and Methods for Modeling of Crystallization Processes," **U.S. Patent No. 8,315,842**, November 20, 2012.
6. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a Conceptual Segment," **C.N. Patent No. 101310282A**, April 25, 2012
7. 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.
8. S. Wang, Y. Song, C.-C. Chen, "Extension of COSMO-SAC Solvation Model for Electrolytes," US Patent Application No.: 20120095736, April 19, 2012.
9. 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.
10. C.-C. Chen, "Computer Method and System for Predicting Physical Properties Using a

Conceptual Segment Model," US Patent Application No.: 20110257947, October 20, 2011.

11. 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.

12. 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.

13. 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.

14. 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.

15. L. Zong, S. Ramanathan, C.-C. Chen, "System and Method of Modeling Triglycerides in Biodiesel Feedstock," US Patent Application No.: 20100280810 A1, November 2010.

16. 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.

17. 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.

18. 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.

19. 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.

20. 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.

21. 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.

22. 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)

Refereed Journal Articles

1. Y. Zhang, C.-C. Chen, "Modeling CO_2 Absorption and Desorption by Aqueous Monoethanolamine Solution with Aspen Rate-Based Model," *Energy Procedia*, in press, 2013

2. 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**, 13792-13802 (2012)

3. B. Hanley, C.-C. Chen, "Useful Mass Transfer Correlations for Packed Towers," *AIChE Journal*, **58**, 132-152 and 2290-2293 (2012); 6 citations

4. 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**, 68-76 (2011); 3 citations

5. 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**, 11406-11421 (2011); 4 citations

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

7. 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**, 190-203 (2011); 2 citations

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

9. 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**, 963-977 (2011); 6 citations

10. Y. Zhang, "Modeling Gas Solubilities in Aqueous Methyldiethanolamine Solution," *Industrial & Engineering Chemistry Research*, **50**, 6436-6446 (2011); 3 citations

11. S. Wang, Y. Song, C.-C. Chen, "Extension of COSMO-SAC Solvation Method for Electrolytes," *Industrial & Engineering Chemistry Research*, **50**, 176-187 (2011); 2 citations

12. Y. Zhang, C.-C. Chen, "Thermodynamic Modeling of CO_2 Absorption in Aqueous Methyldiethanolamine Solution with Electrolyte NRTL Model," *Industrial & Engineering Chemistry Research*, **50**, 163-175 (2011); 14 citations

13. 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); 5 citations

14. 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**, 5479-5484 (2010); 8 citations

15. 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**, 876-886 and 3022-3023 (2010); 6 citations

16. Y. Zhang, H. Chen, J. Plaza, R. Dugas, G. Rochelle, C.-C. Chen, "Rate-Based Process Modeling Study of CO_2 Capture with Aqueous MEA Solution," *Industrial & Engineering Chemistry Research*, **48**, 9233-9246 (2009); 31 citations

17. Y. Song, C.-C. Chen, "Symmetric Electrolyte Nonrandom Two-Liquid Activity Coefficient Model," *Industrial & Engineering Chemistry Research*, **48**, 7788-7797 (2009); 25 citations

18. Y. Song, C.-C. Chen, "Symmetric Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes," *Industrial & Engineering Chemistry Research*, **48**, 5522-5529 (2009); 3 citations

19. S. Wang, S. Watanasiri, S.-T. Lin, C.-C. Chen, "Use of GAMESS/COSMO Program in

Support of COSMO-SAC Model Applications in Phase Equilibrium Prediction Calculations," *Fluid Phase Equilibria*, **276**, 38-46 (2009); 6 citations

20. L.D. Simoni, J.F. Brennecke, M.A. Stadtherr, C.-C. Chen, "Correlation and Prediction of Phase Behavior of Organic Compounds in Ionic Liquids Using NRTL-SAC," *Industrial & Engineering Chemistry Research*, **47**, 7081-7093 (2008); 14 citations

21. G.M. Bollas, C.-C. Chen, P.I. Barton, "Refined Electrolyte-NRTL Model: Activity Coefficient Expressions for Application to Multi-Electrolyte Systems," *AIChE Journal*, **54**, 1608-1624 (2008); 15 citations

22. P.B. Kokikar, E. Plocharczyk, C.-C. Chen, "Modeling Drug Molecule Solubility to Identify Optimal Solvent Systems for Crystallization," *Organic Process Research & Development*, **12**, 249-256 (2008); 9 citations

23. H.-H. Tung, J. Tabora, N. Variankaval, D. Bakken, C.-C. Chen, "Prediction of Pharmaceutical Solubility via NRTL-SAC and COSMO-SAC," *Journal of Pharmaceutical Sciences*, **97**, 1813-1820 (2008); 21 citations

24. S. Wang, C.-C. Chen, S.I. Sandler, "Refinement of COSMO-SAC and the Applications," *Industrial & Engineering Chemistry Research*, **46**, 7275-7288 (2007); 44 citations

25. C.-C. Chen, P.A. Crafts, "Correlation and Prediction of Drug Molecule Solubility in Mixed Solvent Systems with the Non-Random Two-Liquid Segment Activity Coefficient (NRTL-SAC) Model," *Industrial & Engineering Chemistry Research*, **45**, 4816-4824 (2006); 35 citations

26. C.-C. Chen, P.A. Crafts, "Correlation and Prediction of Drug Molecule Solubility with the NRTL-SAC Model," *Computer Aided Chemical Engineering*, **21**, Part 1, 859-864 (2006)

27. E. Mullins, R. Oldland, Y.A. Liu, S. Wang, S.I. Sandler, M. Zwolak, K.C. Seavey, C.-C. Chen, "Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods," *Industrial & Engineering Chemistry Research*, **45**, 4389-4415 (2006); 58 citations

28. C.-C. Chen, "Toward Development of Activity Coefficient Models for Process and Product Design of Complex Chemical Systems," *Fluid Phase Equilibria*, **241**, 103-112 (2006); 15 citations

29. C.-C. Chen, Y. Song, "Extension of NonRandom Two-Liquid Segment Activity Coefficient Model for Electrolytes," *Industrial & Engineering Chemistry Research*, **44**, 8909-8921 (2005); 15 citations

30. C.-C. Chen, Y. Song, "Solubility Modeling with NonRandom Two-Liquid Segment Activity Coefficient Model," *Industrial & Engineering Chemistry Research*, **43**, 8354-8362 (2004); 46 citations

31. L.T. Novak, Y. Song, C.-C. Chen, "Segment-Based Eyring-NRTL Viscosity Model for Mixtures Containing Polymers," *Industrial & Engineering Chemistry Research*, **43**, 6231-6237 (2004); 29 citations

32. K.C. Seavey, Y.A. Liu, T. Lee, N.P. Khare, B. Lucas, J. Pettrey, T.N. Williams, J. Mattson, C. Larkin, E. Schoenborn, C.-C. Chen, "New Mass-Transfer Model for Simulating Industrial Nylon-6 Production Trains," *Industrial & Engineering Chemistry Research*, **43**, 5063-5076 (2004); 4 citations

33. Y. Song, C.-C. Chen, "Generalized Electrolyte NRTL Model for Mixed-Solvent Electrolyte Systems," *AIChE Journal*, **50**, 1928-1941 (2004); 37 citations

34. N.P. Khare, B. Lucas, K.C. Seavey, Y.A. Liu, A. Sirohi, S. Ramanathan, Y. Song, S. Lingard, C.-C. Chen, "Steady State and Dynamic Modeling of Gas-Phase Polypropylene Processes Using Stirred-Bed Reactors," *Industrial & Engineering Chemistry Research*, **43**,

884-900 (2004); 26 citations

35. K.C. Seavey, N.P. Khare, Y.A. Liu, T. Bremner, C.-C. Chen, "Quantifying Relationships among Molecular Weight Distribution, Non-Newtonian Shear Viscosity, & Melt Index for Linear Polymers," *Industrial & Engineering Chemistry Research*, **42**, 5354-5362 (2003); 13 citations

36. K.C. Seavey, N.P. Khare, Y.A. Liu, T.N. Williams, C.-C. Chen, "A New Phase-Equilibrium Model for Simulating Nylon-6 Polymerization Processes," *Industrial & Engineering Chemistry Research*, **42**, 3900-3913 (2003); 10 citations

37. Y. Song, P.M. Mathias, D.A. Tremblay, C.-C. Chen, "Liquid Viscosity Model for Polymer Solutions and Mixtures," *Industrial & Engineering Chemistry Research*, **42**, 2415-2422 (2003); 23 citations

38. S. Behme, G. Sadowski, Y. Song, C.-C. Chen, "A Multicomponent Flash Algorithm for Mixtures Containing Polydisperse Polymers," *AIChE Journal*, **49**, 258-268 (2003); 13 citations

39. N.P. Khare, K.C. Seavey, Y.A. Liu, S. Ramanathan, S. Lingard, C.-C. Chen, "Steady-State and Dynamic Modeling of Commercial Slurry High-Density Polyethylene (HDPE) Processes," *Industrial & Engineering Chemistry Research*, **41**, 5601-5618 (2002); 30 citations

40. P.M. Mathias, N. Orbey, C.-C. Chen, "Hasan Orbey-An Exceptional Applied Thermodynamicist and A Special Friend," *Industrial & Engineering Chemistry Research*, **41**, 5, 885-886 (2002)

41. E. L. Cheluget, C. P. Bokis, L. Wardhaugh, J. Fisher, C.-C. Chen, "Modeling Polyethylene Fractionation Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State," *Industrial & Engineering Chemistry Research*, **41**, 968-988 (2002); 26 citations

42. C.-C. Chen, P.M. Mathias, Applied Thermodynamics for Process Modeling, *AIChE Journal*, **48**, 194-200 (2002); 44 citations

43. C.-C. Chen, C.P. Bokis, P.M. Mathias, "Segment-Based Excess Gibbs Energy Model for Aqueous Organic Electrolyte Systems," *AIChE Journal*, **47**, 2593-2602 (2001); 18 citations

44. C.-C. Chen, P.M. Mathias, H. Orbey, "Use of Hydration and Dissociation Chemistries with the Electrolyte NRTL Model," *AIChE Journal*, **45**, 1576-1586 (1999); 36 citations

45. C.P. Bokis, H. Orbey, C.-C. Chen, "A Segment Contribution Method for the Vapor Pressure of Tall-Oil Chemicals," *Fluid Phase Equilibria*, **155**, 193-203 (1999); 10 citations

46. C.P. Bokis, H. Orbey, C.-C. Chen, "Properly Model Polymer Processes," *Chemical Engineering Progress*, **95**, 39-52 (1999); 20 citations

47. H. Orbey, C.P. Bokis, C.-C. Chen, "Equation of State Modeling of Phase Equilibrium in the Low-Density Polyethylene Process: The Sanchez-Lacombe, Statistical Associating Fluid Theory, and Polymer-Soave-Redlich-Kwong Equations of State," *Industrial & Engineering Chemistry Research*, **37**, 4481-4491 (1998); 35 citations

48. H. Orbey, C.P. Bokis, C.-C. Chen, "An Extension of Cubic Equations of State to Vapor-Liquid Equilibria in Polymer-Solvent Mixtures," *Fluid Phase Equilibria*, **145**, 169-192 (1998); 18 citations

49. H. Orbey, C.P. Bokis, C.-C. Chen, "Polymer-Solvent Vapor-Liquid Equilibrium: Equations of State versus Activity Coefficient Models," *Industrial & Engineering Chemistry Research*, **37**, 1567-1573 (1998); 24 citations

50. C.-C. Chen, Molecular Thermodynamic Model for Gibbs Energy of Mixing of Nonionic Surfactant Solutions, *AIChE Journal*, **42**, 3231-3240 (1996); 15 citations

51. J. King, D.I.C. Wang, C.-C. Chen, "A Molecular Thermodynamic Model for Helix-Helix Docking and Protein Aggregation," *AIChE Journal*, **41**, 1015-1024 (1995); 12 citations

52. C.-C. Chen, "A Segment-Based Local Composition Model for the Gibbs Energy of Polymer Solutions," *Fluid Phase Equilibria*, **83**, 301-312 (1993); 115 citations

53. C.-C. Chen, Y. Zhu, J. King, L.B. Evans, "Molecular Thermodynamic Model to Predict the α-Helical Secondary Structure of Polypeptides Chains in Solution," *Biochemistry*, **31**, 10591-10601 (1992); 9 citations

54. C.-C. Chen, Y. Zhu, J. King, L.B. Evans "A Molecular Thermodynamic Approach to Predict the Secondary Structure of Homo-polypeptides in Aqueous Systems," *Biopolymers*, **32**, 1375-1392 (1992); 24 citations

55. G.H. Ko, M.M. Osias, D.T. Tremblay, M.D. Barrera, C.-C. Chen, "Process Simulation in Polymer Manufacturing," *Computers & Chemical Engineering*, **16**, S481-S490 (1992)

56. I. Farag, P.C. Wu, J.B. Rosen, C.-C. Chen, "Modeling Pollution Prevention," *ChemTech*, **22**, 54-62 (1992); 2 citations

57. D. Austgen, G.T. Rochelle, C.-C. Chen, "Model of Vapor-Liquid Equilibria for Aqueous Acid Gas-Alkanolamine Systems. II. Representation of H_2S and CO_2 Solubility in Aqueous MDEA with MEA or DEA," *Industrial & Chemical Engineering Research*, **30**, 543-555 (1991); 140 citations

58. Y. Zhu, L.B. Evans, C.-C. Chen, "Representation of Phase Equilibrium Behavior of Antibiotics," *Biotechnology Progress*, **6**, 266-272 (1990); 16 citations

59. M. Modell, P. Evanich, S. Anavi, J. Mai, C.-C. Chen, "The Role of Computerized Modeling and Simulation in the Development of Life-Support System Technologies," *Advances in Space Research*, **9**, 121-131 (1989)

60. Y. Zhu, L.B. Evans, C.-C. Chen, "Phase Partitioning of Biomolecules: Solubilities of Amino Acids," *Biotechnology Progress*, **5**, 111-118 (1989); 60 citations

61. D. Austgen, G.T. Rochelle, P. Xiao, C.-C. Chen, "A Model of Vapor-Liquid Equilibria in the Aqueous Acid Gas-Alkanolamine System Using the Electrolyte NRTL Equation," *Industrial & Chemical Engineering Research*, **28**, 1060-1073 (1989); 165 citations

62. C.-C. Chen, "Some Recent Developments in Process Simulation for Reactive Chemical Systems," *Pure & Applied Chemistry*, **59**, 1177-1188 (1987); 4 citations

63. B. Mock, L.B. Evans, C.-C. Chen, "Thermodynamic Representation of Phase Equilibria in Mixed-Solvent Electrolyte Systems," *AIChE Journal*, **32**, 1655-1664 (1986); 218 citations

64. C.-C. Chen, "Representation of Solid-Liquid Equilibrium of Aqueous Electrolyte Systems with the Electrolyte NRTL Model," *Fluid Phase Equilibria*, **27**, 457-474 (1986); 22 citations

65. C.-C. Chen, L.B. Evans, "Local Composition Model for the Excess Gibbs Energy of Aqueous Electrolyte Systems," *AIChE Journal*, **32**, 444-454 (1986); 413 citations

66. C.-C. Chen, L.B. Evans, J.F. Floess, L. Fong, J.P. Longwell, "Modeling of an Oil Shale Fluidized-Bed Retarding Process Using ASPEN," *Energy Progress*, **2**, 147-150 (1982)

67. C.-C. Chen, J.F. Boston, H.I. Britt, L.B. Evans, "Local Composition Model for the Excess Gibbs Energy of Electrolyte Systems - Part I: Single Solvent, Single Completely Dissociated Electrolyte Systems," *AIChE Journal*, **23**, 588-596 (1982); 431 citations

68. C.-C. Chen, J.F. Boston, H.I. Britt, L.B. Evans, "Extension and Application of the Pitzer Equation for Vapor-Liquid Equilibrium of Aqueous Electrolyte Systems with Molecular Solutes," *AIChE Journal*, **25**, 820-831 (1979); 93 citations

69. B.A. Solomon, C.K. Colton, C.-C. Chen, "Immobilization of Acetate Kinase on Functional Solid-core Polymeric Beads," *Enzyme Engineering*, **4**, 105-108 (1978)

Non-Refereed Journal Articles

1. C.-C. Chen, "Solubility: Are You Flying Blind?," *Pharmaceutical Manufacturing*, page 30-32, October 2009
2. C.-C. Chen, "An Industry Perspective on Polymer Process Modeling," *CAST Communications*, Summer 2002
3. V.V. de Leeuw, C.-C. Chen, "Fluid Phase Equilibria in Polymer Systems," *Entropie*, **212/213**, 57-64 (1998)
4. T.L. Mock, D.A. Tremblay, C.-C. Chen, "Process Modeling to Optimize PET Plants," *Chemical Fibers International*, **45**, 208-215 (1995)
5. I.H. Farag, P.W. Gallier, C.-C. Chen, "Addressing Hazardous Waste Incineration by Simulation," *Petrochemicals and Refining*, page 12-16, July 1992
6. I.H. Farag, I. Gosling, R.P. Field, C.-C. Chen, "Simulating Wastewater Treatment Processes," *The Chemical Engineer*, **481**, 31-38 (1990)
7. C.-C. Chen, S.C. Moore, T.M. Piper, "Computer Simulation of An Existing Ammonia Plant," *Ammonia Plant Safety*, **26**, 56-62 (1986)
8. C.-C. Chen, J.F. Boston, T.J. Galloway, K.Y. Lee, B. Mock, "Bayer Process Simulation by ASPEN," *Light Metals*, 295-312 (1983)
9. P.W. Gallier, C.-C. Chen, H.I. Britt, L.B. Evans, "ASPEN: Advanced System for Process Engineering," *Perspectives in Computing*, 1, 43-49 (1981)
10. C.-C. Chen, L.B. Evans, "More Computer Programs for Chemical Engineers," *Chemical Engineering*, page 167-173, May 21, 1979
11. C.-C. Chen, J.N. Peterson, L.B. Evans, "Computer Programs for Chemical Engineers: 1978, Part 1," *Chemical Engineering*, page 145-154, June 5, 1978; 4 citations
12. C.-C. Chen, J.N. Peterson, L.B. Evans, "Computer Programs for Chemical Engineers: 1978, Part 2," *Chemical Engineering*, page 69-84, July 3, 1978 ; 5 citations
13. C.-C. Chen, J.N. Peterson, L.B. Evans, "Computer Programs for Chemical Engineers: 1978, Part 3," *Chemical Engineering*, page 79-86, July 31, 1978
14. C.-C. Chen, J.N. Peterson, L.B. Evans, "Computer Programs for Chemical Engineers: 1978, Part 4," *Chemical Engineering*, page 107-115, August 28, 1978; 3 citations

Book Chapters

1. C.-C. Chen, "Molecular Thermodynamics for Pharmaceutical Process Modeling and Simulation," *Chemical Engineering in Pharmaceutical Industry: R&D to Manufacturing,* D.J. Am Ende (editor), John Wiley & Sons, 505-519 (2011)
2. C.-C. Chen, S. Watanasiri, P. Mathias, V. de Leeuw, "Economic Value of Thermodynamics in Industry and Major Unmet Needs of Aspen Clients," *Chemical Thermodynamics for Industry*, T. Letcher, editor, Royal Society of Chemistry, Cambridge, U.K. (2004)
3. C.-C. Chen, K.-D. Hungenberg, F. Zhang, M. Wulkow, G. Stubbe, U. Nieken, "Design of Polymer Processes Using the Coupling of Commercial Simulation Packages Polymers Plus® and PREDICI®," *Dechema-Monographien Band*, **137**, 237-245 (2001)
4. S. Ramanathan, M. Barrera, M. Osias, G. Ko, C.-C. Chen, "Dynamic Flowsheet Simulation of Polymer Manufacturing Plants," *Dechema-Monographien Band*, **127**, 123-132 (1992)

5. C.-C. Chen, J.F. Boston, H.I. Britt, W.M. Clarke, "Thermodynamic Property Evaluation in Computerized Process Design Scheme for Aqueous Electrolyte Systems," *AIChE Symposium Series,* No. **229**, v.79, 126-134 (1983)
6. C.-C. Chen, J.F. Boston, H.I. Britt, L.B. Evans, "Application of the Extended Pitzer Equation and the Local Composition Model to the Vapor-Liquid Equilibrium of the NH_3-CO_2-H_2S-H_2O System*,*" *ACS Symposium Series Supplement*, **133**, 77-98 (1980)
7. C.-C. Chen, J.F. Boston, H.I. Britt, L.B. Evans, "Two New Activity Coefficient Models for the Vapor-Liquid Equilibrium of Electrolyte Systems," *ACS Symposium Series*, **133**, 61-89 (1980)

Conference Proceedings

1. 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
2. C.-C. Chen, Y. Song, D.A. Tremblay, C. Bhat, "A Rate-Based Process Modeling Study of CO2 Capture with Aqueous Amine Solutions Using aspenONE Process Engineering," *Proceedings 33rd International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference")*, Clearwater, Florida, June 1-5, 2008
3. C.-C. Chen, P.A. Crafts, "Correlation and Prediction of Drug Molecule Solubility with the NRTL-SAC Model," *Proceedings of 16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering*, 859-864 (2006)
4. C.-C. Chen, S. Oba, T. Suzuki, S. Anavi, H. Chen, J.-J. Peng, H.-L. Li, "RateSep – A New and Innovative Rate-Based Distillation Model for Amine Acid Gas Treating Processes," *Proceedings of 4th International Symposium on Molecular Thermodynamics and Molecular Simulation*, Chiba, Japan, May 23-25, 2006
5. C.-C. Chen, H.-H. Tung, N. Variankaval, J. Tabora, D. Bakken, "Prediction of Pharmaceuticals Solubility via NRTL-SAC and COSMO-SAC," *Proceedings of 16th International Symposium on Industrial Crystallization,* Dresden, Germany, September 11-14, 2005 (VDI Berichte, Issue 1901 I, 2005, Article number A-47, Pages 271-276)
6. C.-C. Chen, H.I. Britt, V. Mahalec, A. McBrien "Modeling and Simulation in 2004: An Industrial Perspective," *Proceedings of FOCAPD 2004, Sixth International Conference on Foundations of Computer Aided Process Design*, 55-68 (2004)
7. C.-C. Chen, S. Oba, P.M. Mathias, and Y. Song, "Phase Equilibrium Predictions and Applications with COSMO Solvation Models," *Proceedings of 3rd International Symposium on Molecular Thermodynamics and Molecular Simulation,* Sendai, Japan, May 27-30, 2003
8. P.M. Mathias, M. Walters, C.-C. Chen, "Modeling the Complex Chemical Reactions and Mass Transfer in a Phosphoric Acid Reactor," *Proceedings of 3rd Joint China/USA Chemical Engineering Conference,* 04-218 – 04-225 (2000)
9. C.-C. Chen, C.P. Bokis, E. Cheluget, J. Fisher, L. Wardhaugh, "Modeling Polyethylene Fractionation Using the Statistical Associating Fluid Theory," P*roceedings of 3rd Joint China/USA Chemical Engineering Conference,* 05-032 – 05-041 (2000)
10. C.-C. Chen, B. Mock, L.B. Evans, "Phase Equilibria in Multiple-Solvent Electrolyte Systems: A New Thermodynamic Model," *Proceedings of 1984 Summer Computer*

Simulation Conference, 558-562 (1984)

11. C.-C. Chen, J.F. Boston, H.I. Britt, "Process Simulation of Electrolyte Systems," Proceedings of 1984 Summer Computer Simulation Conference, 552-557 (1984)

12. P.W. Gallier, J.F. Boston, H.I. Britt, L.B. Evans, C.-C. Chen, "New Capabilities in ASPEN PLUS," *Proceedings of the Systems Simulation Symposium of Fossil Fuel Conversion Processes*, 57-68 (1984)

13. P.W. Gallier, H.I. Britt, L.B. Evans, C.-C. Chen, "ASPEN PLUS, the Process Simulator," *Proceedings of Summer 1982 Simulation Conference*, 473-478 (1982)

Invited Lectures

1. Invited lecture at Seventh Joint China/USA Chemical Engineering Conference, Beijing, China, October 14-18, 2013

2. *Molecular Thermodynamics and Process Modeling Technology for Energy and the Environment*, Maddox Distinguished Lecture Series, Texas Tech University, Lubbock, Texas, September 25, 2012

3. *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

4. *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

5. *Process Modeling and Simulation for Energy and the Environment: An Industry Perspective*, Shenghau NICE Advisory Board Meeting, Pasadena, California, February 24-26, 2011

6. *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

7. *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

8. *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

9. *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

10. *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

11. *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

12. *A Journey of Learning in Process Modeling and Simulation*, EPISTAR lecture presentation at Chemical Engineering Department, National Tsinghua University, Taiwan, April 10, 2009

13. *Applied Thermodynamics for Process Modeling: History, Applications, Challenges and Opportunities,* EPISTAR lecture presentation at Chemical Engineering Department, National Tsinghua University, Taiwan, April 8, 2009

14. *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

15. *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

16. *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

17. *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

18. *Recent Advances in Modeling and Simulation for Product and Process Development*, presented at the Chemical Engineering Department, Zhejiang University, Hangzhou, China, May 26, 2008

19. *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

20. *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

21. *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

22. *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

23. *Recent Advances in Modeling and Simulation for Product and Process Development*, paper presented at the PSE China Conference, Xian, China, August 15-18, 2007

24. *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.

25. *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

26. *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

27. *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

28. *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

29. *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

30. *Polymer Process Modeling*, paper presented at BASF Symposium on Modeling and Simulation for Polymer Product and Process Development," Ludwigshafen, Germany, May 1997

31. *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

32. *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

33. *Industrial Applications of Process Simulators,* invited lecture at the Taipei International Chemical Industrial Show Conference, Taipei, Taiwan, August 25-30, 1989

34. *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

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

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

3. *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

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

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

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

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

8. *Development of a Segment-Based DEPG Physical Solvent Model for CO₂ Capture Processes*, presented at the 35th International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference"), Clearwater, Florida, June 6-10, 2010

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

10. *Electrolyte NRTL Model for Thermodynamic Representation of CO₂ Absorption in Aqueous Monoethanolamine and 2-Amino-2-methyl-1-propanol Solutions,* with Y. Zhang, presented at the Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

11. *Development of a DEPG-Based CO₂ Capture Process Model*, with L. Zong, presented at the Properties and Phase Equilibria for Product and Process Design 2010 Conference, Suzhou, China, May 16-21, 2010

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

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

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

15. *Modeling and Simulation in Support of Quality by Design*, paper presented at the AIChE Annual Meeting, Nashville, TN., November 8-13, 2009

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

17. *What's New: Aspen Solubility* Modeler, paper presented at Aspen Worldwide User Conference, Houston, Texas, May 4-7, 2009

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

19. *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, paper presented at the AIChE Annual Meeting, Philadelphia, Pennsylvania, November 16-21, 2008

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

21. *A Rate-Based Process Modeling Study of CO₂ Capture with Aqueous Amine Solutions Using aspenONE process Engineering*, presented at the 33rd International Technical Conference on Coal Utilization & Fuel Systems ("The Clearwater Coal Conference"), Clearwater, Florida, June 1-5, 2008

22. *AspenTech Research Initiatives*, presented at the China User Group Meeting, Hangzhou, China, May 27-28, 2008

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

24. *Rate-Based CO_2 Capture Solvent Packages in aspenONE 2006.5*, presented at the Japan User Group Meeting, Tokyo, Japan, May 20-21, 2008

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

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

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

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

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

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

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

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

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

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

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

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

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

38. *Product Direction for AspenONE Process Modeling – Chemicals*, paper presented at China User Group Meeting, Shanghai, China. May 25-26, 2006
39. *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, paper presented at the 4th International Symposium on Molecular Thermodynamics and Molecular Simulation, Chiba, Japan, May 23-25, 2006
40. *Solubility Prediction of Pharmaceuticals in Pure and Mixed Solvents with NRTL-SAC,* with Peter A. Crafts, paper presented at Aspen Engineering User Group Meeting, Amsterdam, The Netherlands, November 7-8, 2005
41. *Estimating Solubility of Organic Salts with eNRTL-SAC Model*, with Y. Song, paper presented at the AIChE Annual Meeting, Cincinnati, OH, October 30 - November 1, 2005
42. *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, paper presented at Aspen Engineering User Group Meeting, Houston, TX, October 24-25, 2005
43. *Prediction of Pharmaceuticals Solubility via NRTL-SAC and COSMO-SAC,* with Hsien-Hsin Tung, Nara Variankaval, Jose Tabora, and Daniel Bakken, paper presented at the 16th International Symposium on Industrial Crystallization, Dresden, Germany, September 11-14, 2005
44. *Solubility Modeling with the Non-Random Two-Liquid Segment Activity Coefficient Model,* paper presented at the 2nd Annual CHI Predictive ADME Conference, San Diego, CA, January 10-11, 2005
45. *A Practical Phase Equilibrium Model for Solvent Selection in Pharmaceutical Industry – Organic Electrolytes*, with Y. Song, paper presented at the AIChE Annual Meeting, Austin, TX, November 7-12, 2004
46. *Solubility Modeling and Design of Crystallization Processes*, with J.E. Tabora, H.-H. Tung, D. Bakken, and Yuhua Song, paper presented at ASPENWOLRD 04, Orlando, Florida, October 10-15, 2004
47. *Viscosity Model for Mixtures Containing Polymers*, with Lawrence T. Novak and Yuhua Song, paper presented at ASPENWOLRD 04, Orlando, Florida, October 10-15, 2004
48. *Polymer Thermodynamics for Process Modeling*, with Y. Song, paper presented at the AIChE National Meeting, New Orleans, LA, April 25-29, 2004
49. *AspenTech's Engineering Solutions for Chemicals and Polymers*, paper presented at the AspenTech China 2003 Information Technology Forum & User Group Meeting, Beijing, China, December 3-4, 2003
50. *A Practical Phase Equilibrium Model for Solvent Selection in Pharmaceutical Industry*, paper presented at the AIChE Annual Meeting, San Francisco, CA, November 16-21, 2003
51. *Polymers Plus Development Directions,* with D.A. Tremblay, paper presented at the AspenTech User Group Meeting, New Orleans, LA, October 5-8, 2003, and Paris, France, October 19-22, 2003
52. *A Generalized Electrolyte NRTL Model for Mean Ionic Activity Coefficients of Mixed-Solvent Electrolyte Systems*, paper presented at the AspenTech User Group Meeting, Paris, France, October 19-22, 2003
53. *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, paper presented at the AspenTech

User Group Meeting, New Orleans, LA, October 5-8, 2003, and Paris, France, October 19-22, 2003

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

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

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

57. *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, paper presented at the AIChE Annual Meeting, Indianapolis, IN., November 3-8, 2002

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

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

60. *Polymers Plus – A Status Report*, paper presented at ASPENWORLD 02, Washington, D.C., October 27-November 1, 2002

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

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

63. *Simulation of Electrolyte Processes - Status and Challenges,* with P. M. Mathias, paper presented at the AIChE Spring Meeting, New Orleans, LA, March 10-14, 2002

64. *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, paper presented at the AIChE Annual Meeting, Reno, NV, November 4-9, 2001

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

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

67. *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, paper presented at the AIChE Spring National Meeting, Houston, TX, April 22-26, 2001

68. *A Segment-Based Excess Gibbs Energy Model for Aqueous Organic Electrolyte Systems*, with C.P. Bokis and P.M. Mathias, paper presented at the AIChE Annual Meeting, Los

Angeles, CA, November 13-17, 2000

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

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

71. *Development and Application of HDPE Reaction Simulation Model*, paper presented at Aspen World China, Beijing, China, July 13-14, 2000

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

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

74. *Physical Properties and Phase Equilibria in Polymer Process Simulation*, with C.P. Bokis and H. Orbey, paper presented at the AIChE National Meeting, Houston, TX, March 14-18, 1999

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

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

77. *Design, Control, and Optimization of Polymerization Processes,* with T. Mock, paper presented at Chemputers IV Conference, Houston, Texas, March 1996

78. *A Phase-Equilibrium Model for Semi-Crystalline Polymers,* with D. Embry, paper presented at the AIChE Spring National Meeting, New Orleans, February 25-29, 1996

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

80. *AspenTech Polymers Technology Program,* paper presented at ASPENWORLD 94, Boston, MA. November 6-9, 1994

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

82. *Computer Modeling of Chemical Processes with Electrolytes,* paper presented at the Symposium on Basic Chemistry for Industrial Applications, ACS National Meeting, Washington, D.C., August 21-25, 1994

83. *Thermodynamic Analysis in Protein Aggregation and Protein Refolding,* paper presented at the 7th Annual BPEC Symposium on Protein Processing & Protein Interactions, MIT, Cambridge, Mass., November 23-24, 1992

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

85. *Application of Simulation to Agrichemical Processes,* with D. Denholm, Pao-Chen Wu, paper presented at the AIChE Annual Meeting, Miami Beach, FL, 1992

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

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

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

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

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

91. *Simulation of Polymer Processes with Aspen Plus^{TM}*, with G.H. Ko, M. Barrera, D.A. Tremblay, and M. Oasia, paper presented at ACHEMA 91, Frankfurt am Main, Germany, June 9-15, 1991

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

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

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

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

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

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

98. *Application of Aspen Plus in Simulation of High Pressure Tubular Polyethylene Reactor,* with G.H. Ko and S. Anavi, paper presented at the AIChE National Meeting, Orlando, FL., March 1990

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

100. *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, paper presented at the AIChE Spring Meeting, Houston, TX, 1989

101. *Applications Modeling Project Execution,* paper presented at AspenTech Japan User Group Meeting, Kyoto, Japan, 1989

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

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

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

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

106. *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, paper presented at the AIChE Spring Meeting, New Orleans, LA, 1988

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

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

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

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

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

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

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

114. *Process Simulation of Metallurgical Processes,* with H.J. Herzog, J.D. Lenoir and L. Crabs, paper presented at the Benelux Process Control in Metallurgy Symposium, Brussels, Belgium, May, 1986

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

116. *Computer Simulation of an Existing Ammonia Plant,* with S.C. Moore and T.M. Piper, paper presented at the 1985 AIChE Ammonia Safety Symposium, Seattle, August 25-28, 1985

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

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

119. *Computer-Aided Engineering of Electrolyte Systems,* with L.B. Evans, paper presented at the AIChE Annual Meeting, San Francisco, CA, November 25-30, 1984

120. *Process Simulation of Electrolyte Systems,* with H.I. Britt and J.F. Boston, paper presented at the 1984 Summer Computer Simulation Conference, Boston, MA, July 23-25, 1984

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

122. *Bayer Process Simulation by ASPEN*, with J.F. Boston, T.J. Galloway, K.Y. Lee and B. Mock, paper presented at the AIChE Meeting, Anaheim, CA, April 1984

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

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

125. *Bayer Process Simulation by ASPEN*, with J.F. Boston, T.J. Galloway, K.Y. Lee and B. Mock, paper presented at the AIME Meeting, Atlanta, GA, March 1983

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

127. *ASPEN Electrolyte Simulation Capabilities,* with J.F. Boston, H.I. Britt, and L.B. Evans, paper presented at the AIChE National Meeting, Houston, TX, April 1981

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