

RICHARD L. ROWLEY

Personal Curriculum Vitae

Professor of Chemical Engineering, Dept. of Chem. Eng., 350 CB, Brigham Young University, Provo, UT 84602
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POSITIONS

5/1/2007 – Present Chair, Department of Chemical Engineering, Brigham Young University, Provo, UT
9/1/2006 – 5/1/2007 Associate Dean of Engineering and Technology, Brigham Young University, Provo, UT
9/1/89 – Present Professor, Dept. of Chemical Engineering, Brigham Young University, Provo, UT
9/1/95 – 9/1/2000 James J. Christensen Professor of Chemical Eng., Brigham Young University, Provo, UT
8/1/90 – 8/31/95 Chair, Department of Chemical Engineering, Brigham Young University, Provo, UT
1/1/84 – 8/31/89 Associate Professor, Dept. of Chemical Engineering, Brigham Young University, Provo, UT
7/1/83 – 12/31/83 Associate Professor, Dept. of Chemical Engineering, Rice University, Houston, TX
8/15/78 – 7/1/83 Assistant Professor, Dept. of Chemical Engineering, Rice University, Houston, TX

EDUCATION

Ph.D. [1978] - Physical Chemistry, Michigan State University, East Lansing, MI
B.S. [1974] - Chemistry, Magna Cum Laude, Brigham Young University, Provo, UT

PROFESSIONAL DEVELOPMENT

Sep. 1989 - Jun 1990: National Institute of Standards and Technology, Boulder, CO
"Nonequilibrium Molecular Dynamics Simulations of Structured Fluids"
Feb 1998 - May 1998: University of Joensuu, Joensuu, Finland, "Ab Initio Calculations of Intermolecular Potentials"

INDUSTRIAL EXPERIENCE

Thermophysical Property Prediction, Engineering Dept., Texaco, Inc. - [1981]

HONORARY AND PROFESSIONAL SOCIETIES

American Chemical Society (ACS)
American Institute of Chemical Engineers (AIChE)
Phi Kappa Phi
Sigma Xi

PROFESSIONAL SERVICE

AIChE Task Committee for Molecular Modeling [1997-2002]
Joint Committee on Thermo Physical Properties (AIChE/ASME) – [2006 – present]

APPOINTMENTS AND AWARDS

Stand and Deliver Award (selected by college-wide student vote) – [2005]
University Sponsored Research Award - [2001]
College Teacher Award - [1998]
BYU Maeser Research and Creative Arts Award - [1997]
Teacher of the Year Award, Student Alumni Association - [1994, 1997, 1998]
James J. Christensen Research Professorship - [1995-2000]
College of Engineering Outstanding Faculty Award - [1990]
BYU Engineering College New Faculty Research Fellowship - [1987-88]
George R. Brown Superior Teaching Award - [May 1983]
ARCO Outstanding Junior Faculty Member Award - [July, 1981]
Sigma Xi Award for Meritorious Research - [May 4, 1978]
General Electric summer fellowship for outstanding research - [1978]

RESEARCH EXPERTISE

Thermophysical properties: prediction, correlation, evaluation, and database compilation
Molecular dynamics and Monte Carlo simulations of fluids and fluid properties
Simulation, prediction, and measurement of liquid mixture transport properties
Statistical Mechanics

PAST RESEARCH SUPPORT

Government support of research from NSF-ENG, NSF-CPE, DOE, INEL, and NSF-CBT from 1978 - 2005: 9 projects, \$738,000.
Private Support from Welch Foundation, ACS, GPA, GRI, and AIChE from 1978 - 2005: 3 projects, \$506,000.
Corporate Support from Texaco, Wiltec, Koch, Dow, 3M, Conoco, Neste from 1978 - 2000: 9 projects, \$300,000.
NSF Engineering Education grants from 1997-2000: 2 projects (joint with 5 other PIs from

other universities), \$678,000.

CURRENT RESEARCH SUPPORT AIChE DIPPR Project 801: "Evaluated Database", \$300,000/year [1998-continuing]
AIChE DIPPR Database Dissemination Contract, Variable amount/year (\$70,000/year is an expected average) [1998-indefinite]

GRAD. STUDENT WORK DIRECTED
PhD Dissertations

1. W. M. Clark, "Diffusion Measurements Near Critical Mixing Points in Binary and Ternary Liquid Systems," 1984
2. I. C. Wei, "A Local Composition Model for Liquid Mixture Shear Viscosity," 1984
3. J. R. Battler, "Liquid-Liquid Equilibrium Surfaces from Binary Heats of Mixing," 1984
4. W. V. Wilding, "A Four-Parameter Corresponding States Method for Prediction of Thermodynamic Properties of Polar and Nonpolar Fluids," 1985
5. S. Yi, "A Systematic Experimental Investigation of Heats of Transport and Heat-Mass Onsager Coefficients via the Diffusion Thermoeffect," 1987
6. J. Stoker, "Experimental and Molecular Dynamics Simulation Studies of Liquid Mutual Diffusion Coefficients," 1989
7. N. Giles, "Prediction of Mixture Excess Properties from Molecular Dynamics Simulations," 1991
8. P. Crozier, "OMD Simulations of Activity Coefficients in Mixtures," 2001
9. Y. Yang, "NEMD Simulations of Synthetic Lubricants," 2001
10. B. Goodman, "Thermodynamic Property Prediction for Solid Organic Compounds Based on Molecular Structure," 2003.

MS Theses

1. G. E. Platt, "Diffusion Thermoeffect in Ternary Liquid Mixtures," 1980
2. E. R. Peterson, "Thermal Diffusion Near a Binary Liquid Azeotrope," 1981
3. T. Vongvanich, "Heat of Transport in Toluene-Chlorobenzene-Bromobenzene Mixtures," 1982
4. M. D. Hall, "The Diffusion Thermoeffect in Binary Liquid Mixtures," 1984.
5. G. L. White, "Measuring the Thermal Conductivity of Ternary Organic Liquid Systems Using a New Hot-Wire Thermal Conductivity Apparatus," 1986.
6. S. Chandrasekhar, "Heats of Transport in Nonideal Binary Liquid Mixtures," 1986.
7. M. Chiu, "Ternary Liquid Mixture Thermal Conductivity," 1986
8. K. Johnson, "Properties of Fluid Mixtures Containing Polar Components from Four-Parameter Corresponding States: Predictive Mixing Rules for Vapor-Liquid Equilibria," 1987.
9. M. Hanks, "Mathematical Model for the Shape of the Melt/Solid Interface During Horizontal Bridgman Growth of Compound Semiconductor Crystals," 1988.
10. K. Okeson, "A Four-Parameter Corresponding-States Method for Prediction of Newtonian, Pure-Component Viscosity," 1989.
11. V. Gubler, "A Transient Hot-Wire Cell for Measurement of Fluid Thermal Conductivity over a Wide Range of Temperatures and Pressures," 1989.
12. R. Powles, "Vapor-Liquid Equilibrium Measurements on Selected Binary Mixtures," 1991.
13. E. Johansen, "Transient Hot-Wire Cells for Measurement of Thermal Conductivities of Gases and Liquids," 1992.
14. Stephen Gill, "Removal of Semi-Volatile Fission Products," 1995.
15. Darin Anderson, "A Absorption of CO₂ into aqueous alkanolamine solutions," 1996.
16. M. Michael Painter, "Transport Property Equations of State for the Lennard-Jones Fluid from Molecular Dynamics Simulations," 1996.
17. Matthew Henrichsen, "Osmotic Molecular Dynamics Simulations of Chemical Potential for Structured Molecules," 1996.
18. William Allen, "NEMD Simulations of Viscosity of Structured Molecules," 1997.
18. Mike Adams, "Absorption of CO₂ into Aqueous Alkanolamine Solutions," 1997.
19. Norman Fuller, "NEMD Simulations of the viscosity of Polar Structured Molecules," 1998.
20. Erik Ericksen, "OMD Simulations of Mixtures of Structured Molecules," 1999.
21. H. Wang, "Molecular Simulation of Equilibrium and Dynamic Properties at the Liquid-Liquid Interface," 2003.

BS Honor Theses

1. E. Carlson, "Molecular Dynamics Simulation of the Liquid-Liquid Interface of a Partially

Miscible Mixture," 2003.

**CURRENT GRAD.
STUDENTS**

1. Jason Thomas, "Simulation of fluid viscosity using transient molecular dynamics simulations", Ph.D. <April 2008>
2. Jiangping Liu, "Fluid dipole moments and dielectric constant", Ph.D. <April 2009>

**UNIVERSITY
SERVICE**

Department Chair (2007-present)
Associate Dean of Engineering & Technology for Strategic Planning (25%, 2005-2007)
Department Undergraduate Committee (1978-80, 84-90, 99-2007)
University Graduate Council (1982-83, 1999-2003)
University Department Review Committee (1999-2003)
Department Graduate Committee (1981-83, 85-90)
College Advancement in Rank Committee (1988-89; 1995-1997)
Departmental Public Relations (1983-90)
Department Chair (1990-1995)
University FAC Council (1997-1999)
Department Undergraduate Committee Chair (1998-1999; 2004-2006)

PUBLICATIONS

A. Books and Monographs

1. R.L. Rowley, The Diffusion Thermoeffect in Binary Liquid Mixtures, Ph.D. Dissertation, Michigan State University, 1978.
2. R.L. Rowley, The First Law of Thermodynamics, AIChE CHEME Module D5.2, (AIChE, New York, 1985).
3. J.J. Christensen, R.L. Rowley and R.M. Izatt, Handbook of Heats of Mixing. Supplementary Volume, John Wiley & Sons, New York (1988).
4. R.L. Rowley, "Application on Nonequilibrium Thermodynamics to Heat and Mass Transport Properties: Measurement and Prediction in Nonelectrolyte Liquid Mixtures" in *Flow, Diffusion, and Rate Processes*. Advances in Thermodynamics Series Vol. 6, S. Sieniutycz and P. Salamon, eds. (Taylor & Francis, New York, 1992).
5. R.L. Rowley, *Statistical Mechanics for Thermophysical Property Calculations*, Prentice-Hall, Englewood Cliffs, New Jersey (1994).
6. R.L. Rowley, *Statistical Mechanics for Thermophysical Property Calculations: Solutions Manual*, Prentice-Hall, Englewood Cliffs, New Jersey (1995).
7. R. L. Rowley, *Molecular Modeling and Thermophysical Properties*, nearing completion.
8. R. L. Rowley and W.V. Wilding, "Section 2: Prediction and Correlation of Physical Properties" in *Perry's Handbook, Eighth Edition*, McGraw-Hill (to be published in 2007).

B. Peer-Reviewed Journal Publications

1. R.L. Rowley and F.H. Horne, "The Dufour Effect. II. Experimental Confirmation of the Onsager Heat-Mass Reciprocal Relation for a Binary Liquid Mixture", *J. Chem. Phys.* **68**, 325 (1978).
2. R.L. Rowley and F.H. Horne, "The Dufour Effect. III. Direct Experimental Determination of Heats of Transport for the Carbon Tetrachloride-Cyclohexane System", *J. Chem. Phys.* **72**, 131 (1980).
3. R.L. Rowley and F.H. Horne, "The Behavior of the Heat of Transport Near the Critical Solution Temperature of Isobutyric Acid-Water Mixtures", *J. Chem. Phys.* **71**, 3841 (1979).
4. R.L. Rowley, "A Local Composition Model for Multicomponent Liquid Mixture Thermal Conductivities", *Chem. Eng. Sci.* **37**, 897 (1982).
5. G. Platt, T. Vongvanich, and R.L. Rowley, "The Diffusion Thermoeffect in Ternary, Nonelectrolyte Liquid Mixtures", *J. Chem. Phys.* **77**, 2113 (1982).
6. G. Platt, G. Fowler, T. Vongvanich, and R.L. Rowley, "Diffusion Thermoeffect Measurements of Heats of Transport in Ternary Liquid Toluene-Chlorobenzene-Bromobenzene Mixtures at 25 °C and 35 °C", *J. Chem. Phys.* **77**, 2121 (1982).
7. R.L. Rowley, "A Local Composition Model for Thermal Conductivity in Multicomponent Liquid Mixtures", in Proceedings of the 17th International Conference of Thermal Conductivity, J.G. Hust, Ed., pp. 31-44 (Pergamon Press, 1983).
8. G. Platt, G. Fowler, T. Vongvanich, and R.L. Rowley, "Heat-Mass Onsager Coefficients in Ternary Nonelectrolyte Liquid Mixtures", *J. Noneq. Thermo.* **8**, 1 (1983).
9. I.C. Wei and R.L. Rowley, "Binary Liquid Mixture Viscosities and Densities", *J. Chem. Eng. Data* **29**, 332 (1983).
10. I.C. Wei and R.L. Rowley, "Ternary Liquid Mixture Viscosities and Densities", *J. Chem. Eng. Data* **29**, 336 (1983).
11. E. Peterson, T. Vongvanich, and R.L. Rowley, "Thermal Diffusion Factors Near the Azeotrope Conditions of

- Ethanol-Water Mixtures", *J. Chem. Eng. Data* **29**, 6 (1984).
12. R.L. Rowley and J.R. Battler, "Local Composition Models and Thermodynamic Consistency: Prediction of Binary Liquid-Liquid Binodal Curves from Heats of Mixing", *Fluid Phase Equilibria* **18**, 111 (1984).
 13. I.C. Wei and R.L. Rowley, "A Local Composition Model for Multicomponent Liquid Mixture Shear Viscosity", *Chem. Eng. Sci.* **40**, 401 (1985).
 14. J.R. Battler, W.M. Clark, and R.L. Rowley, "Excess Enthalpy and Liquid-Liquid Equilibrium Surfaces for the Cyclohexane-Isopropanol-Water System from 293.15 K to 323.15 K", *J. Chem. Eng. Data* **30**, 254 (1985).
 15. J.R. Battler and R.L. Rowley, "Excess Enthalpies Between 293 K and 323 K for the Constituent Binary Systems of Ternary Mixtures Exhibiting Partial Miscibility", *J. Chem. Thermodynamics* **17**, 719 (1985).
 16. W.M. Clark and R.L. Rowley, "Ternary Liquid Diffusion Coefficients Near Plait Points", *Int. J. Thermophys.* **6**, 631 (1985).
 17. W.M. Clark and R.L. Rowley, "The Mutual Diffusion Coefficient of Methanol-n-Hexane Near the Consolute Point", *AIChE J.* **32**, 1125 (1986).
 18. J.R. Battler and R.L. Rowley, "Prediction of Ternary Liquid-Liquid Equilibria from Excess Enthalpies", *Fluid Phase Equilibria* **25**, 129 (1986).
 19. W.V. Wilding and R.L. Rowley, "A Four-Parameter Corresponding States Method for the Prediction of Thermodynamic Properties of Polar and Nonpolar Fluids", *Int. J. Thermophys.* **7**, 525 (1986).
 20. R.L. Rowley and M.D. Hall, "Heats of Transport from the Diffusion Thermoeffect in Binary Liquid Mixtures of Toluene, Chlorobenzene, and Bromobenzene", *J. Chem. Phys.* **85**, 3550 (1986).
 21. R.L. Rowley and G.L. White, "Thermal Conductivities of Ternary Liquid Mixtures", *J. Chem. Eng. Data* **32**, 63 (1987).
 22. R.L. Rowley, S.C. Yi, V. Gubler, and J.M. Stoker, "Mutual Diffusivity, Thermal Conductivity, and Heat of Transport in Binary Liquid Mixtures of Alkanes in Carbon Tetrachloride", *Fluid Phase Equilib.* **36**, 219 (1987).
 23. W.V. Wilding, J.K. Johnson, and R.L. Rowley, "Thermodynamic Properties and Vapor Pressures of Polar Fluids from a Four-Parameter Corresponding States Method", *Int. J. Thermophys.* **8**, 717 (1987).
 24. S.C. Yi and R.L. Rowley, "Heats of Transport from Diffusion Thermoeffect Measurements on Binary Liquid Mixtures of Carbon Tetrachloride with Benzene, Toluene, 2-Propoanone, n-Hexane, and n-Octane", *J. Chem. Phys.* **87**, 7208 (1987).
 25. S.C. Yi and R.L. Rowley, "On the Use of a Modified Square-Well Model for Prediction and Correlation of Thermal Diffusion Factors in Binary Liquid Mixtures," *J. Chem. Phys.* **87**, 7214 (1987).
 26. R.L. Rowley and V. Gubler, "Thermal Conductivities in Seven Ternary Liquid Mixtures at 40 °C and 1 atm", *J. Chem. Eng. Data* **33**, 5 (1988).
 27. R.L. Rowley, G.L. White, and M. Chiu, "Ternary Liquid Mixture Thermal Conductivities", *Chem. Eng. Sci.* **43**, 361 (1988).
 28. R.L. Rowley, S.C. Yi, D.V. Gubler, and J.M. Stoker, "Mutual Diffusivity, Thermal Conductivity, and Heat of Transport in Binary Liquid Mixtures of Alkanes in Chloroform", *J. Chem. Eng. Data* **33**, 362 (1988).
 29. J. K. Johnson and R.L. Rowley, "Prediction of Vapor-Liquid Equilibria in Binary Mixtures Containing Polar Components from an Extended Lee-Kesler Corresponding States Technique", *Fluid Phase Equilib.* **44**, 255 (1989).
 30. J. K. Johnson and R.L. Rowley, "Application of an Extended Lee-Kesler Corresponding-States Technique to Prediction of Vapor-Liquid Equilibria in Multicomponent Mixtures Containing Polar Components", *Int. J. Thermophys.* **10**, 479 (1989).
 31. S.C. Yi and R.L. Rowley, "Measurement of Heats of Transport in Ternary Liquid Mixtures via the Diffusion Thermoeffect", *J. Nonequilib. Thermodyn.* **14**, 293 (1989).
 32. J.M. Stoker and R.L. Rowley, "Molecular Dynamics Simulation of Real-Fluid Mutual Diffusion Coefficients with the Lennard-Jones Potential Model", *J. Chem. Phys.* **91**, 3670 (1989).
 33. R.L. Rowley, J.L. Oscarson, P.N. Slater, N.F. Giles, and R.M. Izatt, "Molecular-Dynamics Simulations of Excess Enthalpies in Mixtures of Supercritical Carbon Dioxide and Neopentane", *Fluid Phase Equilib.* **53**, 167 (1989).
 34. J.R. Battler and R.L. Rowley, "Excess Enthalpy of Four Partially Miscible Binary Liquid Mixtures near Their Critical Solution Temperatures", *J. Chem. Eng. Data* **35**, 334 (1990).
 35. K.J. Okeson and R.L. Rowley, "A Four-Parameter Corresponding-States Method for Prediction of Newtonian, Pure-Component Viscosity", *Int. J. Thermophys.* **12**, 119 (1991).
 36. R.L. Rowley, J.L. Oscarson, N.F. Giles, W.K. Tolley and R.M. Izatt, "Experimental and Molecular-Dynamics Simulated Excess Enthalpies and Solubilities of Neopentane in Supercritical Carbon Dioxide", *Fluid Phase Equilib.* **60**, 143 (1990).
 37. R.L. Rowley and G.L. Hoffman, "DIPPR Project 805 NSF(B)/88: Vapor Liquid Equilibrium Measurements on Mixtures Important to Industrial Design", *AIChE Symposium Series No. 279* **18**, 6 (1990).
 38. R.L. Rowley, J.M. Stoker and N.F. Giles, "Molecular Dynamics Simulation of Mutual Diffusion in Nonideal Liquid

- Mixtures", *Int. J. Thermophys.* **12**, 501 (1991).
39. R.L. Rowley and J.F. Ely, "Nonequilibrium Molecular Dynamics Simulations of Structured Molecules. I. Isomeric Effects on the Viscosity of Butanes", *Mol. Phys.* **72**, 831 (1991).
 40. R.L. Rowley and J.F., "Nonequilibrium Molecular Dynamics Simulations of *n*-Butane and Isobutane Viscosity", *Molec. Simulation* **7**, 303 (1991).
 41. R. L. Rowley and R. H. Powell, "Vapor-Liquid Equilibrium Measurements on Mixtures Important to Industrial Design - DIPPR Project 805 NSF(B)/89", *DIPPR Data Series No. 1*, 47 (1991).
 42. R.L. Rowley and J.F. Ely, "Nonequilibrium Molecular Dynamics Simulations of Structured Molecules. II. Structural Effects on the Viscosity of Model C₆ Hydrocarbons", *Mol. Phys.* **75**, 713 (1992).
 43. R.L. Rowley and J.F. Ely, "Note on the Number Dependence of Nonequilibrium Molecular Dynamics Simulations of the Viscosity of Structured Molecules", *J. Chem. Phys.* **96**, 4814 (1992).
 44. N.F. Giles, J.L. Oscarson, R.L. Rowley, W.K. Tolley, R.M. Izatt, "Thermodynamic Properties of Mixing for SnCl₄ Dissolved in Supercritical CO₂: A Combined Experimental and Molecular Dynamics Study", *Fluid Phase Equilibria* **73**, 267 (1992).
 45. L.C. Wilson, W.V. Wilding, G.M. Wilson, R.L. Rowley, V.M. Felix and T.Chisolm-Carter, "Thermophysical Properties of HFC-125", *Fluid Phase Equilibria* **80**, 167 (1992).
 46. R.L. Rowley, T.D. Shupe and M.W. Schuck, "A Direct Method for Determination of Chemical Potential with Molecular Dynamics Simulations. Part 1. Pure Components", *Mol. Phys.* **82**, 841 (1994).
 47. R.L. Rowley, T.D. Shupe and M.W. Schuck, "A Direct Method for Determination of Chemical Potential with Molecular Dynamics Simulations", *Fluid Phase Equilib.* **104**, 159 (1995).
 48. R.L. Rowley and R.H. Powell, "Vapor-Liquid Equilibrium Measurements on Mixtures Important to Industrial Design", in Experimental Results for DIPPR 1990-91 Projects on Phase Equilibria and Pure Component Properties; DIPPR Data Series, 2, 116 (1994).
 49. R.L. Rowley, J. Perry and M.W. Schuck, "A Direct Method for Determination of Chemical Potential with Molecular Dynamics Simulations. Part 2. Mixtures", *Mol. Phys.* **86**, 125 (1995).
 50. R.L. Rowley, M.E. Adams, T.L. Marshall, J.L. Oscarson, W.V. Wilding, and D.J. Anderson, "Measurement of Diffusion Coefficients Important in Modeling the Absorption Rate of Carbon Dioxide into Aqueous N-Methyldiethanolamine", *J. Chem. Eng. Data* **42**, 310 (1997).
 51. W. Allen and R.L. Rowley, "Predicting the viscosity of alkanes using nonequilibrium molecular dynamics: Evaluation of intermolecular potential models", *J. Chem. Phys.* **106**, 10273 (1997).
 52. J.N. Harb, A. Jones, R.L. Rowley, and W.V. Wilding, "Use of Computational Tools in Engineering Education: A Case Study on the use of Mathcad at Brigham Young University", *Chem. Eng. Ed.*, Summer 1997, 180.
 53. M. Lahtela, T. Pakkanen, and R.L. Rowley, "Nonequilibrium Molecular Dynamics Simulations of 3-Methylhexane: The Effect of Inter- and Intramolecular Potential Models on Simulated Viscosity", *J. Phys. Chem. A* **101**, 3449 (1997).
 54. D.M. Duh, D. Henderson, and R.L. Rowley, "Some Effects of Deviations from the Lorentz-Berthelot Combining Rules for Mixtures of Lennard-Jones Fluids", *Molec. Phys.* **91**, 1143 (1997).
 55. D.R. Wheeler, N.G. Fuller, and R.L. Rowley, "Nonequilibrium Molecular Dynamics Simulation of the Shear Viscosity of Liquid Methanol: Adaptation of the Ewald Sum to Lees-Edwards Boundary Conditions", *Molec. Phys.* **92**, 55 (1997).
 56. R.L. Rowley and M.M. Painter, "Diffusion and Viscosity Equations of State for a Lennard-Jones Fluid Obtained from Molecular Dynamics Simulations", *Int. J. Thermophys.* **18**, 1109 (1997).
 57. M. Henrichsen and R.L. Rowley, "Chemical Potentials of Structured Molecules from Osmotic Molecular Dynamics Simulations", *Fluid Phase Equilib.* **137**, 75 (1997).
 58. R.L. Rowley, M.E. Adams, T.L. Marshall, J.L. Oscarson, W.V. Wilding, and D.J. Anderson, "Measurement of Diffusion Coefficients Important in Modeling the Absorption Rate of Carbon Dioxide into Aqueous Diethanolamine," *J. Chem. Eng. Data* **43**, 427 (1998).
 59. M. Lahtela, M. Linnolahti, T. Pakkanen, and R.L. Rowley, "Computer Simulation of Branched Alkanes: The effect of side chain and its position on rheological behavior", *J. Chem. Phys.* **108**, 2626 (1998).
 60. M.E. Adams, T.L. Marshall and R.L. Rowley, "Diffusion Coefficients Significant in Modeling the Absorption Rate of Carbon Dioxide into Aqueous Blends of N-Methyldiethanolamine and Diethanolamine and of Hydrogen Sulfide into Aqueous N-Methyldiethanolamine", *J. Chem. Eng. Data* **43**, 605 (1998).
 61. D.R. Wheeler and R.L. Rowley, "Shear viscosity of polar liquid mixtures via non-equilibrium molecular dynamics: water, methanol, and acetone", *Molec. Phys.* **94**, 555 (1998).
 62. N.G. Fuller and R.L. Rowley, "Nonequilibrium Molecular Dynamics Simulation of Shear Viscosity of Polar Liquids", *Int. J. Thermophys.* **19**, 1039 (1998).
 63. W. V. Wilding, R. L. Rowley, and J. L. Oscarson, "DIPPR Project 801 evaluated process design data", *Fluid Phase Equilib.* **150-151**, 413 (1998).

64. R. L. Rowley and T. Pakkanen, "Determination of a methane intermolecular potential model for use in molecular simulations from ab initio calculations", *J. Chem. Phys.* **110**, 3368 (1999).
65. D. Boda, D. Henderson, R. Rowley, and S. Sokolowski, "Simulation and density functional study of a simple membrane separating two restricted primitive model electrolytes", *J. Chem. Phys.* **111**, 9382 (1999).
66. N.G. Fuller and R.L. Rowley, "The Effect of Model Internal Flexibility Upon NEMD Simulations of Viscosity", *Int. J. Thermophys.* **21**, 45 (2000).
67. Y. Yang, T. Pakkanen and R.L. Rowley, "Nonequilibrium Molecular Dynamics Simulations of Shear Viscosity: Isoamyl Alcohol, n-Butyl Acetate and Their mixtures", *Int. J. Thermophys.* **21**, 703 (2000).
68. P.S. Crozier, R.L. Rowley, E. Spohr, and D. Henderson, "Comparison of charged sheets and corrected 3-D Ewald calculations of long-range forces in slab geometry electrolyte systems with solvent molecules", *J. Chem. Phys.* **112**, 9253 (2000).
69. P.S. Crozier, R.L. Rowley, D. Henderson, and D. Boda, "A corrected 3D Ewald calculation of the low effective temperature properties of the electrochemical interface", *Chem. Phys. Lett.* **325**, 675 (2000).
70. P.S. Crozier, R.L. Rowley, and D. Henderson, "Molecular dynamics calculations of the electrochemical properties of electrolyte systems between charged electrodes", *J. Chem. Phys.* **113**, 9202 (2000).
71. T.A. Knotts, W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Use of the DIPPR Database for Development of QSPR Correlations: Surface Tension", *J. Chem. Eng. Data* **46**, 1007-1012 (2001).
72. P.S. Crozier, R.L. Rowley, N.B. Holladay, D. Henderson, and D.D. Busath, "Molecular Dynamics Simulation of Continuous Current Flow Through a Model Biological Membrane Channel", *Phys. Rev. Lett.* **86**, 2467 (2001).
73. R.L. Rowley, Y. Yang, and T.A. Pakkanen, "Determination of an ethane intermolecular potential model for use in molecular simulations from ab initio calculations", *J. Chem. Phys.* **114**, 6059 (2001).
74. P.S. Crozier, R.L. Rowley, and D. Henderson, "Molecular dynamics simulations of ion size effects on the fluid structure of aqueous electrolyte systems between charged electrodes", *J. Chem. Phys.* **114**, 7513 (2001).
75. D. Henderson, D.D. Busath, R.L. Rowley, P.S. Crozier, and D. Boda, "Simulation study of channels in biological membranes", *Proceedings of the International Conference on Computational Nanoscience*, pp. 45-48 (2001).
76. R. J. Rowley, J. L. Oscarson, R. L. Rowley, and W. V. Wilding, "Development of an Automated SMILES Pattern Matching Program To Facilitate the Prediction of Thermophysical Properties by Group Contribution Methods", *J. Chem. Eng. Data*, **46**, 1110-1113 (2001).
77. D. Henderson, D. D. Busath, and R. Rowley, "Fluids near surfaces and in pores and membrane channels", *Progress in Surface Science*, **68**(7-8), 279-295 (2001).
78. P.S. Crozier, D. Henderson, R.L. Rowley, and D.D. Busath, "Model Channel Ion Currents in NaCl-SPC/E Solution with Applied-Field Molecular Dynamics", *Biophys. J.* **81**, 3077-3089 (2001).
79. P.S. Crozier and R.L. Rowley, "Liquid mixture activity coefficient prediction via osmotic molecular dynamics," *AIChE Symp. Series* **325**, 163 (2001).
80. J.-P. Jalkanen, R. Mahlanen, T.A. Pakkanen, and R.L. Rowley, "Ab initio potential energy surfaces of propane dimer", *J. Chem. Phys.* **116**, 1303-1312 (2002).
81. Y. Yang, D. Henderson, P. Crozier, R.L. Rowley, and D.D. Busath, "Permeation of ions through a model biological channel: Effect of periodic boundary conditions and cell size", *Molec. Phys.* **100**, 3011-3019 (2002).
82. P.S. Crozier and R.L. Rowley, "Activity coefficient prediction by osmotic molecular dynamics", *Fluid Phase Equilib.* **193**, 53-73 (2002).
83. Y. Yang, T. A. Pakkanen, and R.L. Rowley, "NEMD simulations of viscosity and viscosity index for lubricant-size model molecules", *Int. J. Thermophys.* **23**, 1441-1454 (2002).
84. D. Ericksen, W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Use of the DIPPR database for development of QSPR Correlations: Normal Boiling Point", *J. Chem. Eng. Data* **47**, 1293-1302 (2002).
85. J.-P. Jalkanen, T.A. Pakkanen, Y. Yang, and R.L. Rowley, "Interaction energy surfaces of small hydrocarbon molecules", *J. Chem. Phys.* **118**, 5474 (2003).
86. H. Wang, E. Carlson, D. Henderson, and R. L. Rowley, "Molecular dynamics simulation of the liquid-liquid interface for immiscible and partially miscible mixtures", *Molec. Simulation* **29**, 777-785 (2003).
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 96. B. T. Goodman, W. V. Wilding, J. L. Oscarson, and R. L. Rowley "A Note on the Relationship Between Organic Solid Density and the Liquid Density at the Triple Point," *J. Chem. Eng. Data* **49**(6), 1512-1514 (2004).
 97. A. C. Vawdrey, J. L. Oscarson, R. L. Rowley, and W. V. Wilding, "Vapor-phase association of n-aliphatic carboxylic acids," *Fluid Phase Equilib.* **222-223**, 239-245 (2004).
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 99. K. E. Wardle, D. J. Henderson, and R. L. Rowley, "Molecular Dynamics Simulation of Surfactant Effects on Ion Transport Through a Liquid-Liquid Interface Between Partially Miscible Liquids," *Fluid Phase Equilib.* **233**, 96-102 (2005).
 100. R. J. Hulse, R. L. Rowley, and W. V. Wilding, "Transient nonequilibrium molecular dynamic simulations of thermal conductivity: 1. simple fluids," *Int. J. Thermophys.* **26**(1), 1-11 (2005).
 101. C. G. Guymon, R. L. Rowley, J. N. Harb, and D. R. Wheeler, "Simulating an electrochemical interface using charge dynamics," *Condensed Matter Phys.* **8**(2), 1-21 (2005).
 102. A. J. Karttunen, R. L. Rowley, and T. A. Pakkanen, "Ab initio study on adsorption of hydrated Na⁺ and Cu⁺ cations on the Cu(111) surface," *J. Phys. Chem. B* **109**, 23983-23992 (2005).
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 104. R. L. Rowley, C. M. Tracy, and T. A. Pakkanen, "Potential energy surfaces for small alcohol dimers I: Methanol and ethanol," *J. Chem. Phys.* **125**, 154302 (2006).
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 106. R.L. Rowley, W.V. Wilding, J.L. Oscarson, and Y. Yang, "Database Tools for Evaluating Thermophysical Property Data," *Int. J. Thermophys.* **28**, 805-823 (2007).
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 110. C. Guymon, J. Harb, R. L. Rowley, and D. Wheeler, "MPSA Effects on Copper Electrodeposition Investigated by Molecular Dynamics Simulations," *J. Chem. Phys.* (accepted Nov 2007).

C. Partially-reviewed & General Papers

111. R.L. Rowley, A Chemical Engineering: Meeting the world-wide challenges of product and process development, @ Engineering Horizons, 32 (1992).
112. M. Lahtela-Kakkonen, T.A. Pakkanen, and R.L. Rowley, ASimulations of Branched Alkanes with Nonequilibrium Molecular Dynamics: Looking for low cost raw materials for quality oils, @ CSC News, 3, 1998.
113. R. L. Rowley, Book Reviw of ATransport Properties of Fluids: Their Correlation, Prediction and Estimation@, J. Chem. Thermodyn. 30, 397 (1998).
114. P.T. Cummings, H.D. Cochran, J.J. dePablo, D.J. Evans, D. Kofke, A.Z. Panagiotopoulos, A. Z. and Rowley, R. L., "A World Wide Web Based Textbook on Molecular Simulation," 1998 American Society of Engineering Education (ASEE) Annual Conference & Exposition, June 28-July 1, 1998. (Available on the web at <http://www.asee.org/conferences/search/00636.PDF>.)

115. J.N. Harb, R.L. Rowley, S.P. Magleby and A.R. Parkinson, "Going Global: Implementation of a College-wide Initiative To Prepare Engineering and Technology Students for the 21st Century," Proceedings of the 2007 Annual ASEE Conference, AC 2007-2912, Honolulu, HI, June (2007).

SEMINARS AND SPEECHES

1. Invited presentation at the DOE Conference on Thermodynamics Research Requirements on Fossil Fuel Processes, Tulsa, OK - June 20, 1979.
2. AIChE 87th National Meeting, "Temperature Dependence of the Heat of Transport Near the Critical Solution Temperature of the Isobutyric Acid-Water System", paper 54c, Boston, MA - August 22, 1979.
3. Seminar, "Transport Phenomena Near Liquid-Liquid Critical Points", University of Texas, Austin, TX - Apr 22, 1980.
4. Seminar, "Prediction of Mixture Transport Properties in Liquids from Thermodynamics", University of Kansas, Lawrence, KA - December 9, 1980.
5. AIChE National Meeting, "Prediction of Liquid Mixture Thermal Conductivities Based on the NRTL Thermodynamic Theory of Mixtures", Paper 43f, Houston, TX - April 9, 1981.
6. International Joint Conferences on Thermophysical Properties, "Prediction of Multicomponent Liquid Mixture Thermal Conductivities", Gaithersburg, MA - June 15, 1981.
7. Seminar, "The Heat Flux in Multicomponent Liquid Mixtures", University of Wyoming, Laramie, WY - Jan. 29, 1982.
8. Seminar, "Prediction of Liquid Mixture Thermal Conductivity and Shear Viscosity", Union Carbide Continuing Education, South Charleston, WV - May 5, 1982.
9. AIChE National Mtg., "Heats of Transport and Heat Flow in Ternary Liquid Mixtures", Houston, TX - Mar 29, 1983.
10. Seminar, "Prediction of Multicomponent Liquid Mixture Transport Properties", Brigham Young University, Provo, UT - May 17, 1983.
11. ASME National Meeting. "Prediction of Multicomponent Liquid Mixture Viscosity from Binary Thermodynamic Data", Boston, MA - Nov. 16, 1983.
12. Seminar, "The Marriage of Thermodynamics and Transport Phenomena", Brigham Young University, Provo, UT - January 19, 1984.
13. Joint IUPAC and 39th Calorimetry Conference, "Binary Liquid-Liquid Equilibria, Enthalpies of Mixing, and Thermodynamic Consistency of Liquid Mixture Models", Hamilton, CANADA - Aug 1984.
14. AIChE National Meeting, "Mutual Diffusion Coefficients Near Liquid-Liquid Binodal Curves", Houston, TX - Mar 1985.
15. Ninth Symposium on Thermophysical Properties, "Ternary Liquid Diffusion Coefficients Near Plait Points", Boulder, CO - Jun 1985.
16. Ninth Symposium on Thermophysical Properties, "A Four-Parameter Corresponding States Method for the Prediction of Thermodynamic Properties of Polar and Nonpolar Fluids", Boulder, CO - Jun 1985.
17. Session Chairman, Ninth Symposium on Thermophysical Properties, Boulder CO - Jun 1985.
18. AIChE National Meeting, "Ternary Liquid Mixture Thermal Conductivities", Miami Beach, Florida - Nov 1986.
19. Session Chairman, Fluid Transport Properties I & II, AIChE Annual Meeting, Miami Beach, Florida, Nov 2-7, 1986.
20. Invited Seminar, "Determination of Molecular Heat and Mass Transport Coefficients in Liquid Mixtures via Transient Techniques", Dept. of Chem. Eng., Polytechnic Institute of New York, Brooklyn, NY - Feb 12, 1987.
21. AIChE National Meeting, "Mutual Diffusivity, Thermal Conductivity, and Heat of Transport in Binary Liquid Mixtures of Alkanes in Carbon Tetrachloride", Houston, Texas - Apr 1, 1987
22. Poster presentation, "The Use of Demonstrations in Teaching Transport Phenomena", 1987 Summer School for Chemical Engineering Faculty, North Dartmouth, Massachusetts, Aug 11, 1987.
23. Dept. of Chem. Eng. Seminar, "Molecules in Motion: The Use of Molecular Dynamics to Predict Thermophysical Properties", Brigham Young University, Nov 5, 1987.
24. Dept. of Chem. Eng. Seminar, "Reflections on Teaching Creativity: A Memorial Presentation on Behalf of the Late Dr. James J. Christensen", Brigham Young University, Nov 19, 1987.
25. Dept. of Chemistry Seminar, "Molecules in Motion: The Use of Molecular Dynamics to Predict Thermophysical Properties", Brigham Young University, Jan 28, 1988.
26. Tenth International Symposium on Thermophysical Properties, "Application of an Extended Lee-Kesler Corresponding-States Technique to Prediction of Vapor-Liquid Equilibria in Multicomponent Mixtures Containing Polar Components", Gaithersburg, Maryland, Jun 1988.
27. Fifth International Conference on Fluid Properties & Phase Equilibria for Chemical Process Design, "Molecular-Dynamics Simulation of Excess Enthalpies and Free Energies in Mixtures of CO₂ and Neopentane", Poster presentation, Banff, Alberta Canada, May 3, 1989.
28. AIChE National Meeting, "Equilibrium Molecular Dynamic Simulations of Mutual Diffusion Coefficients for Alkanes in Carbon Tetrachloride and Chloroform", Orlando, Florida, Mar 21, 1990.

29. College of Engineering Outstanding Faculty Award Lecture, "The Attractive Matter of Liquids", Brigham Young University, Apr, 1990.
30. National Institute of Standards and Technology, Thermophysics Division Seminar, "Liquid Viscosity and Molecular Structure: Molecular Dynamics Simulations", Boulder, Colorado, May 24, 1990.
31. AIChE National Meeting, "Nonequilibrium Molecular Dynamics Simulations of Structured Molecules: Isomeric Effects on the Viscosity of Butanes", Chicago, Illinois, Nov 15, 1990.
32. Eleventh Symposium on Thermophysical Properties, "The Effect of Molecular Structure on Viscosity: Nonequilibrium Molecular Dynamics of C6 Model Fluids", Boulder, Colorado, Jun 25, 1991.
33. Department of Chemical Engineering Seminar, University of Utah, "Prediction of Thermophysical Properties Using Molecular Dynamics Simulations", Nov 13, 1993.
34. International Symposium on Molecular Thermodynamics and Molecular Simulation, "A New Method for Direct Calculation of Chemical Potentials using Molecular Dynamics", Kyoto, Japan, Jan 10, 1994.
35. AIChE Spring National meeting, "A New Method for Direct Calculation of Chemical Potential from Molecular Dynamics", Atlanta, Georgia, Apr 18, 1994.
36. GRI/GPA Conference, AHeats of Mixing and Diffusion coefficients in Aqueous Alkanol Amine Solutions@, San Antonio, TX, Mar 10, 1995.
37. Joensuu University, "NEMD Simulations of Structured Molecules", Joensuu, Finland, May 3, 1995.
38. Neste Corporate Technology, "Modeling of Synthetic Lubricants", Helsinki, Finland, May 5, 1995.
39. Seventh International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, "Osmotic Molecular Dynamics Simulations of Lennard-Jones Mixtures", Snowmass/Aspen, CO, Jun 18-23, 1995.
40. Montana State University, "Molecular Dynamics Simulations of Thermophysical Properties", Bozeman, Montana, April 1996.
41. AIChE Fall National Meeting, "NEMD Viscosity Simulations of Models of Linear and Branched Alkanes: The Effect of Structure and Potential Model", speaker: W. Allen, Chicago, Illinois, November, 1996.
42. AIChE Local Section Meeting, "The Maze in Which the Tiny Atoms Run", Provo, UT, March 1997.
43. Thirteenth Symposium on Thermophysical Properties, "Nonequilibrium Molecular Dynamics Simulation of the Shear Viscosity of Polar Liquids", Boulder, CO, June 1997.
50. Thirteenth Symposium on Thermophysical Properties, "DIPPR Project 801: Evaluated Process Design Data", speaker W. Vincent Wilding, Boulder, CO, June 1997.
51. AIChE Fall National Meeting, "Mixture Activity Coefficients from OMD Simulations: An Analog to Group Contribution Methods", Los Angeles, CA, November, 1997.
52. AIChE Fall National Meeting, "NEMD Simulations of Viscosity: Mixtures of Polar Molecules", Los Angeles, CA, November, 1997.
53. MoRa Modelling Conference at VTT Chemical Technology Center, "NEMD Simulations of Viscosity", Helsinki, Finland, February, 1998.
54. MoRa Project Meeting at Neste Oil Company, "Ab initio calculations of intermolecular potential", Helsinki, Finland, April, 1998.
55. Department of Chemistry Seminar, "Calculation of intermolecular potentials from ab initio calculations for use in MD simulations", University of Joensuu, Joensuu, Finland, April, 1998.
56. DIPPR Conference, "Predictions of Properties from Quantum Mechanics", Provo, June 1998.
57. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 37", Provo, June 1998.
58. Department of Chemical Engineering Graduate Seminar, "Calculation of intermolecular potentials from ab initio calculations", BYU, Provo, September 1998.
59. AIChE National Meeting, "Ab initio calculations of intermolecular potentials: C-C, C-H and H-H interactions in methane", paper 771, Miami Beach, November 1998.
60. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 38", AIChE National Meeting, Miami Beach, November 1998.
61. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 39", Provo, Utah, June 1999.
62. DIPPR Conference, "Molecular Simulation and Computational Chemistry", Provo, Utah, June 1999
63. Graduate Student Seminar, "Determination of intermolecular potentials for molecular dynamics simulations from ab initio calculations", Department of Chemical Engineering, University of Nevada, Reno, October 1999.
64. Undergraduate Student Seminar, "The Maze in Which the Tiny Atoms Run", Department of Chemical Engineering, University of Nevada, Reno, October 1999
65. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 40", AIChE National Meeting, Dallas, November 2, 1999.
66. Exxon Research and Engineering Seminar, "Advanced, Molecular-Based, Computational Techniques for Thermophysical Property Estimation", November 16, 1999.

67. Exxon Research and Engineering Seminar, "The DIPPR Advantage in Thermophysical Property Values", November 16, 1999.
68. Fourteenth Symposium on Thermophysical Properties, "Use of the DIPPR database for development of QSPR correlations: Surface Tension", Boulder, May 31, 2000.
69. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 41", Provo, Utah, June 2000.
70. FOMMS 2000, "Prediction of liquid phase activity coefficients from osmotic molecular dynamics simulations", Keystone, Colorado, July 25, 2000.
71. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 42", AIChE National Meeting, Los Angeles, November 12, 2000.
72. Pacifichem 2000, "Simulation of Model Aqueous Electrolytes Near a Charged Surface", Session 114, paper 32, Honolulu, Dec 14, 2000.
73. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 43", Provo, Utah, May 30-31, 2001.
74. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 44", AIChE National Meeting, Reno, NV, Nov. 6, 2001.
75. AIChE National Meeting, "Transferrable Intermolecular Potential Models from Ab Initio Calculations", Session 125, Paper i, Reno, NV, Nov. 7, 2001.
76. AIChE National Meeting, "A Molecular Simulation Module for Teaching Vapor-Liquid Equilibrium", Session 2, Paper c, Reno, NV, Nov. 5, 2001.
77. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 45", Park City, Utah, May 30, 2002.
78. Yangtze International Conference of Fluids and Interfaces, "Molecular dynamics simulations of the liquid-liquid interface", Nanjing to Chongqing, China, October 12-18, 2002.
79. R. L. Rowley, R. J. Rowley, J.L. Oscarson, and W.V. Wilding (speaker), "DIPPR 801 Evaluated Database: The Third Decade," AIChE Spring Meeting, New Orleans, March 2003.
80. B.T. Goodman (speaker), W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Use of the DIPPR Database for the Development of QSPR Correlations: Solid Vapor Pressure and Heat of Sublimation of Organic Compounds", 15th Symposium of Thermophysical Properties, Boulder, CO, June 23, 2003.
81. A.C. Vawdrey (speaker), W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "An examination of vapor-phase association in the n-aliphatic carboxylic acids using density functional theory", 15th Symposium of Thermophysical Properties, Boulder, CO, June 23, 2003.
82. G.J. Smith (speaker), W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Correlation of Liquid Viscosity at the Normal Boiling Point", 15th Symposium of Thermophysical Properties, Boulder, CO, June 25, 2003.
83. R.J. Hulse (speaker), W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Transient Nonequilibrium Molecular Dynamic Simulations of Thermal Conductivity", 15th Symposium of Thermophysical Properties, Boulder, CO, June 25, 2003.
84. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 47", Boulder, CO, June 27, 2003.
85. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 48," AIChE National Meeting, San Francisco, CA, November 17, 2003.
86. R.L. Rowley, "Molecular Simulations of the Liquid-Liquid Interface," Department Graduate Seminar, Brigham Young University, January 14, 2004.
87. K. E. Wardle, E. Carlson, D. Henderson (speaker), and R. L. Rowley, "Molecular dynamics simulation of the effect of ions on a liquid/liquid interface for a partially miscible mixture," NATO Workshop on "Ionic Soft Matter: Novel Trends in Theory and Applications," L'viv, Ukraine, April., 2004.
88. K. E. Wardle (speaker), D. Henderson, and R. L. Rowley, "Molecular Dynamics Simulation of the Transport of Ions Across a Liquid-Liquid Interface (LLI) with a Surfactant," 10th International Conference on "Properties and Phase Equilibria for Product and Process Design" (PPEPPD), Snowbird, Utah, May 17-21, 2004.
89. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 49", Provo, Utah, May 21, 2004.
90. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 50", AIChE National Meeting, Austin, Texas, Nov 8, 2004.
91. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 51", Provo, Utah, June 1, 2005.
92. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 52", AIChE National Meeting, Austin, Texas, Nov 8, 2005.
93. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 53", Salt Lake City, June, 2006.
94. R.L. Rowley, "Database Tools for Evaluating Thermophysical Property Data (Invited Talk)", Thermo International 2006, Boulder, CO, July 31, 2006.
95. J.R. Rowley (speaker), W.V. Wilding, J.L. Oscarson, and R.L. Rowley, "Rapid Evaluation of Prediction Methods with DIPPR's Automated Property Prediction Package", Thermo International 2006, Boulder, CO, July 31, 2006.
96. J.C. Thomas (speaker) and R.L. Rowley, "Transient molecular dynamics simulations of viscosity and thermal diffusivity for simple fluids", Thermo International 2006, Boulder, CO, Aug 1, 2006.

97. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 54", San Francisco, CA, November 3, 2006.
98. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 55," Houston, TX, Apr 23, 2007.
99. J. Thomas and R.L. Rowley (speaker), "Transient Molecular Dynamics Simulation of Viscosity," Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design – PPEPPD 2007, May 20, Poster SIM3, May 22, 2007.
100. DIPPR Conference, "Progress Report of DIPPR Project 801: Report 56", AIChE National Meeting, Salt Lake City, UT, November 8, 2007.

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