

CURRICULUM VITAE

JAMES F. ELY

University Professor Emeritus
Professor, Chemical and Biological Engineering Department
Colorado School of Mines
Golden, CO 80401-1887

Phone: 303-273-3720
Fax: 303-273-3730
Email: jely@mines.edu
<http://inside.mines.edu/~jely>

Education

B.S., *Magna Cum Laude*, Chemistry and Physics, Butler University,
Indianapolis, IN, 1968
Ph.D. Chemical Physics, Indiana University, Bloomington, IN, 1971 (Thesis
Advisor, D. A. McQuarrie)

Postdoctoral Studies

National Research Council - National Academy of Sciences Postdoctoral
Fellow, National Bureau of Standards, Boulder, CO, 11/71 - 11/73 (Advisors, H.
J. M. Hanley and D. Diller)

Chemical Engineering Department, Rice University, Houston, TX, 12/73-4/75
(Advisor, Riki Kobayashi)

Employment History

8/07-1/2013, *Director*, Bioengineering and Life Sciences
Colorado School of Mines, Golden, CO.

8/00-8/10, *Head*, Chemical Engineering Department,
Colorado School of Mines, Golden, CO.

5/01-present, *Director*, Colorado Institute for Energy, Materials and
Computational Science (CIEMACS—formerly CIFER and CCER)), Colorado
School of Mines, Golden, CO.

8/91-present, *Professor*, Chemical Engineering Department,
Colorado School of Mines, Golden, CO. (Tenured, 1994) (*University Professor
Emeritus*, 2011).

1/91-8/91, *Associate Director*, Chemical Science and Technology Laboratory,
National Institute of Standards and Technology, Boulder, CO.

10/88- 8/91, *Group Leader*, Theory of Fluids Group, National Institute of
Standards and Technology, Boulder, CO.

9/81- 5/91, *Adjunct Professor*, Chemical Engineering and Petroleum Refining
Department, Colorado School of Mines, Golden, CO.

7/79-10/88, *Chemist*, National Bureau of Standards, Boulder, CO.

4/77-7/79, *Senior Research Chemist*, Chemical Engineering Department
Corporate R&D Engineering, Shell Development Co., Houston, TX.

4/75-4/77 *Research Chemist*, Chemical Engineering Department, Corporate R&D
Engineering, Shell Development Co., Houston, TX.

- Editorships** 1988 - 1997, *Editor*, Fluid Phase Equilibria (Elsevier Publishers, Amsterdam)
FPE Special Issue Editor, 1987, 1991, 1993, 1998, 2000, 2003
Editorial Board, Fluid Phase Equilibria, 2000-2008
Editorial Board, J. Chem. Eng. Data, 2000-2003
- Professional Societies** American Institute of Chemical Engineers
American Chemical Society
American Physical Society
American Society for Engineering Education
Materials Research Society
- Professional Activities** FOMMS 2006 Organizing Committee Senior Advisor
FOMMS 2003 Meeting Chairman
FOMMS 2000 Organizing Committee
ASEE Summer School Workshop Leader, 2002
CACHE Molecular Modeling Task Force, 1998-present
Organizing Committee, 7th International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, 1995
Local Arrangements Chair, 12th Symposium on Thermophysical Properties, 1994
Session Chairman, 13th European Conference on Thermophysical Properties, Workshop on Phase Equilibria, Lisbon, Portugal, 1993.
Chairman, 11th Symposium on Thermophysical Properties, 1991
ASME Thermophysical Properties K-7 Committee, 1988-present
NBS Research Advisory Committee, 1986-1989
Oak Ridge National Laboratory Technical Evaluation Committee, 1985
Gas Processors Association Data Book Revision Committee, 1984-1985
AIChE DIPPR Advisory Committee, 1983-1985
AIChE Area Ia Program Committee, 1981-1987, 1991 - 1997
(Chairman, 1985-1987)
NBS-NEL Technical Advisory Committee, 1983-1984
AIChE Meeting Session Chairman, 1978, 1984, 1987, 1990-2002
EPRI Coal Liquefaction Technical Steering Committee, 1976-1983
Gas Processors Association Enthalpy Steering Committee, 1976-1979
- Honors** Donald L Katz Award for Research, Gas Processors Association, 2009
Erskine Fellowship, University of Caterbury, 2004
Visiting Scholar, University of New South Wales, 2004
CSM Alumni Association Outstanding Teaching Award, 2002
U.S. Department of Commerce Silver Medal for Meritorious Federal Service, 1986 (Citation: *For outstanding creativity in developing theoretically based predictive models for the thermophysical properties of fluids*)
Federal Laboratory Consortium Special Award for Excellence in Technology Transfer, 1986
NBS Sustained Superior Performance Award, 1983, 1985-1990
NBS Special Act Award, 1985
NBS Outstanding Performance Award, 1981, 1982, 1984
NRC - NAS Research Associate, 1971-1973
NDEA IV Fellow, 1968-1971
University Scholar, Butler University, 1964-1968
- Listings** American Men and Women of Science

**Teaching and
Related
Activities**

Courses Taught at the Colorado School of Mines:

CHEN 200 Computational Methods in Chemical Engineering
CHEN 201 Chemical Process Principles
CHEN 202 Chemical Process Principles Laboratory
CHEN 307 Unit Operations I - Fluid Mechanics
CHEN 308 Unit Operations II - Heat Transfer
CHEN 312/313 Unit Operations Laboratory
CHEN 357 Introduction to Chemical Engineering Thermodynamics
CHEN 358 Chem. Eng. Thermodynamics Laboratory
CHEN 375 Unit Operations III - Mass Transfer
CHEN 420 Mathematical Methods in Chemical Engineering
CHEN 440 Molecular Perspectives in Chemical Engineering
CHEN 505 Numerical Methods in Chemical Engineering
CHEN 507 Applied Mathematics in Chemical Engineering
CHEN 509 Advanced Chemical Engineering Thermodynamics
CHEN 520 Thermodynamics of Phase Equilibrium
CHEN 609 Adv. Topics in Thermodynamics (Computer Simulation)
CHEN 610 Applied Statistical Thermodynamics
CHEN 611 Applied Statistical Mechanics
CHEN 625 Applied Molecular Theory and Simulation
CHGN 351 Physical Chemistry for the Biosciences
EGGN 371 Engineering Thermodynamics
DCGN 210 Distributed Core Thermodynamics
CSM 101 Freshman Success Seminar

Ph. D. Graduate Student Thesis Supervision

1. Dale D. Erickson, *A Method for Improving Equations of State Near the Critical Point*, 1988. (Rice University, co-advised with T. W. Leland)
2. Laurel A. Watts, *The Solubility of ZnO in Supercritical H₂O-NaCl Solutions*, 1994.
3. Jianzhi Ge, *Statistical Mechanical Models for the Properties of Asymmetric Fluid Mixtures*, 1995.
4. Vibha Bansal, *Molecular Dynamics Studies of Rheology in Fluid Mixtures*, 1996.
5. Isabel Marrucho-Ferreira, *Extended Corresponding States Theory: Application for Polar Compounds and Their Mixtures*, 1997. (co-advised with A. M. F. Palavra, University of Lisbon)
6. Jurivan Ratanapisit, *Studies of thermal Transport Properties Using Molecular Dynamics Simulation Techniques*, 1999.
7. Lixin Sun, *Development of Advanced Equations of State for Engineering Application*, 2003
8. Haizhong Zhang, *Simulation Force Fields for Fluid Transport Properties*, 2003.
9. Nuno Galamba, *Equilibrium and Non-equilibrium Molecular Dynamics Simulation of the Transport Coefficients of Molten Alkali Halides*, 2004. (co-advised with C. A. N. DeCastro, University of Lisbon)
10. Bin Liu, *Modeling and Simulation of Hydrocarbon Dissociation on Nickel Surfaces*, 2008 (co-advised with Mark A. Lusk, CSM, Physics)
11. Dawn Culley, *Development of a Universal m-6-8 United Atom Force Field for Molecular Simulation*, 2009
12. John Jechura, *Process Simulation of Bio-mass Conversion Processes*, 2013, (expected)

M.S. Graduate Student Thesis Supervision

1. Joseph D. Kuhach, *A Hard Sphere Expansion Equation of State Applied to Conformal Solution Theory*, 1985.
2. Luis A. Chu, *An Experimental Study of Solubility Differences between Phenol and m-Cresol in Supercritical Carbon Dioxide*, 1986. (co-advised with R. M. Baldwin)
3. Gerald J. Sherman, *Isochoric PVT Experiments for (0.99 CO₂ + 0.01 C₂H₆) and Modeling PVT Behavior of Carbon Dioxide Rich Mixtures*, 1988.
4. Jeffery R. Swanson, *Investigation of Dense Fluid Viscosity by Molecular Dynamics Simulation of Hard Spheres*, 1989
5. Tappan K. Bhatt, *Application of Selection Algorithm Methodology to the Development of New Equations of State for Refrigerants*, 1993.
6. Katherine B. Shubert, *Application of linear regression decision algorithms In the development of equations of state for refrigerants R134a and R123*, 1994.
7. Jurivan Ratanapisit, *Modification of the Lee-Kesler Model Using MBWR-32 Equations of State*, 1995.
8. Bichun Xu, *Mixing Rules and a Corresponding States Model for Refrigerant Mixtures*, 1996
9. Collier, Shawn M. *Determination of Carbon Dioxide Fugacities in Carbon Dioxide + Isobutane Mixtures Using a Hollow Fiber Silica Membrane*, 1997.(co-advised with D. J. Way)
10. Kindra M. Snow, *Development of a Simple, Accurate Equation of State for Alternative Refrigerants*, 1997.
11. Karl Maurer, *The Neo-classical Equation of State: Five-Point Contact Revisited*, 1997.
12. Ratan Mandavilly, *Molecular Scale Flow Visualization Using MD Techniques*, 2000
13. Charity Garrison, *Design and Construction of a Gas Absorber for the Unit Operations Laboratory*, 2003
14. Gina Mabe, *Thermodynamic Property Add-in for Excel*, 2004
15. Brian Dossey, *Modified BWR Equations of State for n-Hexane and n-Dodecane*, 2005
16. Matt Mitchell, *A Virtual Thermodynamics Laboratory*, 2006
17. Heather Barkley, *Coexistence curves from Grand Canonical Monte Carlo Using Different Forcefields*, 2007

**CSM
Committee
Service**

BELS (Bioengineering and Life Sciences) Board of Directors (2003 - 2012),
Chairman (2004 - 2007)
Strategic Plan Recalibration Committee (2007-2008)
CSM Faculty Compensation Committee(2007-2011)
CSM Handbook Committee (2008-2011)
Research Management Council (2007-2011)
SCT Banner Advisory Committee (2005 -2007)
Engineering Division Director Search Committee (2005)
Vice-President for Research Search Committee (2004)
CSM Technology Fee Award Committee (2001 - 2002, 2005 - 2010)
CSM Safety Committee (2001 - 2004)
Department Heads Executive Committee (2000 – 2010)
Materials Science Board of Directors (2000 - present)
CSM Faculty Senate Executive Committee (1999-2000)
CSM Faculty Senate (1994 – 1997, 1999-2000)
Resource and Infrastructure Committee (1994 – 1999, 2002 - 2004)
Curriculum Reform Steering Committee (1994-1997, 2000 - 2004)
Faculty Search Committees (7) (1993, 1995, 1997-1999)
Research Council (1992 - 1994)
Research Plan Committee (1992-1993)

**CSM Research
Funding**

8/91-7/92	Volume Correction Factor for Natural Gas Liquids, Gas Processors Association, \$40,000
8/92-7/95	Composition Dependence of Fluid Thermophysical Properties: Theory and Modeling, U. S. DOE, \$369,000
6/93-5/96	Simulation of Rheology in Hydrocarbon Lubricants, Exxon Foundation, \$30,000
8/95-2/99	Composition Dependence of Fluid Thermophysical Properties: Theory and Modeling, U. S. DOE, \$348,000
7/97-6/02	Computer Aided Chemical Engineering Education, Colorado Commission on Higher Education \$1,417,000
7/97-1/98	A Large Scale Computing Initiative in Chemical Engineering at the Colorado School of Mines, IBM SUR Grant, \$750,000 (with J.D. Way)
8/99-10/02	Composition Dependence of Fluid Thermophysical Properties: Theory and Modeling, U. S. DOE, \$377,927
8/01-8/12	Thermophysical Properties for Renewable Energy, NREL, \$500,000
11/02-10/05	Composition Dependence of Fluid Thermophysical Properties: Theory and Modeling, U. S. DOE, \$405,000
6/03-5/04	Foundations of Molecular Modeling and Simulation FOMMS 2003, NSF-CTS, \$20,000
10/04-9/05	Thermodynamic Evaluation System for Pure and Mixed Chemicals, NIST, \$75,000
8/07-7/10	MRI: Acquisition of a High Performance Computing Cluster Dedicated to the Energy Sciences, NSF-CNS, 8/07-7/10, \$400,000 (with: Lusk, Ganesh, Romig)

Publications

Archival Journal Manuscripts

1. Liu, B.I., M.A. Lusk, and J.F. Ely, *Reactive Molecular Dynamic Simulations of Hydrocarbon Dissociations on Ni(111) Surfaces*, Surface Science, 2012, **606**: 615-623.
2. Liu, B.I., M.A. Lusk, and J.F. Ely, *The influence of nickel catalyst geometry on the dissociation barriers of H₂ and CH₄: Ni₁₃ vs. Ni(111)*. J. Phys. Chem. C, 2009. **113**(31): 13715-13722.
3. Liu, B.I., M.A. Lusk, and J.F. Ely, *Hydrogen Dissociations on Small Nickel Clusters*. Mol. Sim., 2009. **35**(10-11): 928-935.
4. Liu, B.I., et al., *Reactive Molecular Dynamics Force Field for the Dissociation of Light Hydrocarbons on Ni(111)* Mol. Sim., 2008. **34**(10-15): 967-972.
5. Kiselev, S.B. and J.F. Ely, *HRX-SAFT Equation of State for Fluid Mixtures: New Analytical Formulation*. J. Phys. Chem. C, 2007. **111**(43): 15969-15975.
6. Kiselev, S.B. and J.F. Ely, *Generalized crossover description of the thermodynamic and transport properties in pure fluids II. Revision and modifications*. Fluid Phase Equilib., 2007. **252**(1): 57-65.
7. Galamba, N., C.A.N. de Castro, and J.F. Ely, *Equilibrium and nonequilibrium molecular dynamics simulations of the thermal conductivity of molten alkali halides*. J. Chem. Phys., 2007. **126**(20): 4511-4521.
8. Kiselev, S.B., et al., *HRX-SAFT Equation of State for Fluid Mixtures: Application to Binary Mixtures of Carbon Dioxide, Water, and Methanol*. Ind. Eng. Chem. Res., 2006. **45**(11): 3981-3990.
9. Kiselev, S.B., J.F. Ely, and J.R. Elliott Jr., *Molecular Dynamic Simulations and Global Equation of State of Square-Well Fluids with the Well-Widths from $l=1.1$ to 2.1* . Mol. Phys., 2006. **104**(15): 2545-2559.
10. Kiselev, S.B. and J.F. Ely, *A new analytical formulation for the generalized corresponding states model for thermodynamic and surface properties in pure fluids*. Chem. Eng. Sci., 2006. **61**(15): 5107-5113.
11. Sun, L., S.B. Kiselev, and J.F. Ely, *Multiparameter Crossover Equation of State: Generalized Algorithm and Application to Carbon Dioxide*. Fluid Phase Equilib., 2005. **233**(2): 204-219.
12. Sun, L. and J.F. Ely, *A Corresponding States Model for Generalized Engineering Equations of State*. Int. J. Thermophys., 2005. **26**(3): 705-728.
13. Ratanapisit, J.R. and J.F. Ely, *Shear viscosity of hard chain fluids through molecular dynamics simulation techniques*. Songklanakarin J. Sci. Technol., 2005. **27**(4): 847-857.
14. Pan, G., et al., *Operator splitting algorithm for iso-kinetic SLLOD molecular dynamics*. J. Chem. Phys., 2005. **122**(09): 4114-4122.
15. Kiselev, S.B., et al., *Generalized SAFT-DFT/DMT model for the thermodynamic, interfacial, and transport properties of associating fluids: Application for n-alkanols*. Ind. Eng. Chem. Res., 2005. **44**(17): 6916-6927.
16. Galamba, N., C.A.N. de Castro, and J.F. Ely, *Shear viscosity of molten alkali halides from equilibrium and nonequilibrium molecular dynamics simulations*. J. Chem. Phys., 2005. **122**(22): 4501-4509.
17. Abdulagatov, I.M., et al., *Thermodynamic Properties of Methanol in the Critical and Supercritical Regions*. Int. J. Thermophys., 2005. **26**(5): 1327-1368.
18. Abdulagatov, I.M., et al., *PVTx Measurements and Crossover Equation of State of Pure n-Hexane and Dilute Aqueous n-Hexane Solutions in the Critical and Supercritical Regions*. Ind. Eng. Chem. Res., 2005. **44**(6): 1967-1984.
19. Zhang, H. and J.F. Ely, *AUA model NEMD and EMD simulations of the shear viscosity of alkane and alcohol systems*. Fluid Phase Equilib., 2004. **217**(1): 111-118.
20. Sun, L. and J.F. Ely, *Universal equation of state for engineering application: Algorithm and application to non-polar and polar fluids*. Fluid Phase Equilib., 2004. **222-223**(1): 107-118.
21. Kiselev, S.B. and J.F. Ely, *A simplified crossover droplet model for adsorption of pure fluids in slit pores*. J. Chem. Phys., 2004. **120**(17): 8241-52.
22. Kiselev, S.B. and J.F. Ely, *Generalized crossover description of the thermodynamic and transport properties in pure fluids*. Fluid Phase Equilib., 2004. **222-223**(1): 149-159.

23. Galamba, N., C.A.N. de Castro, and J.F. Ely, *Thermal conductivity of molten alkali halides from equilibrium molecular dynamics simulations*. J. Chem. Phys., 2004. **120**(18): 8676-8682.
24. Galamba, N., C.A.N. de Castro, and J.F. Ely, *Molecular dynamics simulation of the shear viscosity of molten alkali halides*. J. Phys. Chem. B, 2004. **108**: 3658-3662.
25. Kiselev, S.B. and J.F. Ely, *Physical Limit of Stability in Supercooled D₂O and D₂O + H₂O mixtures*. J. Chem. Phys., 2003. **118**(2): 680-689.
26. Kiselev, S.B. and J.F. Ely, *Generalized Corresponding States Model for Bulk and Interfacial Properties in Pure Fluids and Fluid Mixtures*. J. Chem. Phys., 2003. **119**(16): 8645-8662.
27. Pai-Panandiker, R.S., et al., *Development of an Extended Corresponding States Principle Method for Volumetric Property Predictions Based on a Lee–Kesler Reference Fluid*. Int. J. Thermophys., 2002. **23**(3): 771-785.
28. Kiselev, S.B., et al., *Computer simulations and crossover equation of state of square-well fluids*. Fluid Phase Equilib., 2002. **200**(1): 121-145.
29. Kiselev, S.B., et al., *Equation of state and thermodynamic properties of pure toluene and dilute aqueous toluene solutions in the critical and supercritical regions*. Ind. Eng. Chem. Res., 2002. **41**(5): 1000-1016.
30. Kiselev, S.B. and J.F. Ely, *Parametric crossover model and physical limit of stability in supercooled water*. J. Chem. Phys., 2002. **116**(13): 5657-5665.
31. Ratanapisit, J.R., D.J. Isbister, and J.F. Ely, *Transport properties of fluids: Symplectic integrators and their usefulness*. Fluid Phase Equilib., 2001. **183**: 351-361.
32. Kiselev, S.B., et al., *A Crossover Equation of State for Associating Fluids*. Fluid Phase Equilib., 2001. **183**: 53-64.
33. Kiselev, S.B. and J.F. Ely, *Curvature effect on the physical boundary of metastable states in liquids*. Physica A, 2001. **299**(3-4): 357-370.
34. Galamba, N., et al., *A corresponding states approach for the calculation of the transport properties of molten alkali halides*. High Temp.-High Pres., 2001. **33**(4): 397-404.
35. Galamba, N., et al., *A corresponding states approach for the calculation of surface tension of molten alkali halides*. Fluid Phase Equilib., 2001. **183-184**: 239-245.
36. Magee, J.W., S.L. Outcalt, and J.F. Ely, *Molar heat capacity, C_v, Vapor Pressure and (p,d,T) measurements from 92 to 350 K at pressures to 35 MPa and a new equation of state for chlorotrifluoromethane*. Int. J. Thermophys., 2000. **21**(5): 1097-1121.
37. Kiselev, S.B., J.F. Ely, and Y.F. Belyakov, *Adsorption of critical and supercritical fluids*. J. Chem. Phys., 2000. **112**(7): 3370-3383.
38. Kiselev, S.B., et al., *Crossover SAFT equation of state and thermodynamic properties of propan-1-ol*. Int. J. Thermophys., 2000. **21**(6): 1373-1405.
39. Kiselev, S.B. and J.F. Ely, *Simplified crossover SAFT equation of state*. Fluid Phase Equilib., 2000. **174**(1/2): 93-113.
40. Baldwin, R.M., et al., *Incorporating molecular modeling into the chemical engineering curriculum*. Chem. Eng. Educ., 2000. **34**(2): 162-168.
41. Ratanapisit, J. and J.F. Ely, *Application of New, Modified BWR Equations of State to the Corresponding States Prediction of Natural Gas Properties*. Int. J. Thermophys., 1999. **20**(6): 1721-1735.
42. Kiselev, S.B. and J.F. Ely, *Crossover SAFT Equation of State: Application for Normal Alkanes*. Ind. Eng. Chem. Res., 1999. **38**(12): 4993-5004.
43. Miller, R.A., et al., *Higher Order Thinking in the Unit Operations Laboratory*. Chem. Eng. Education, 1998. **32**(2): 146.
44. Marrucho, I.M. and J.F. Ely, *Extended Corresponding States for Pure Polar Fluids and Non-Polar Fluids: An Improved Method for Component Shape Factor Prediction*. Fluid Phase Equilib., 1998. **150**: 215-23.
45. Collier, S., et al., *An Apparatus for the Direct Measurement of Fugacity in Mixtures Containing Large and Small Molecules*. Fluid Phase Equilib., 1998. **151**: 807-813.
46. Shubert, K.B. and J.F. Ely, *Application of a new selection algorithm to the development of a wide-range equation of state for refrigerant R134a*. Int. J. Thermophys., 1995. **16**(1): 101-110.
47. Marrucho, I.M., A. Palavara, and J.F. Ely, *An Improved Extended-Corresponding-States Theory for Natural Gas Mixtures*. Int. J. Thermophys., 1994. **15**: 1261-1269.

48. Huber, M.L. and J.F. Ely, *A predictive extended corresponding states model for pure and mixed refrigerants including a new equation of state for R134a*. Int. J. Refrig., 1994. **17**: 18-31.
49. Rowley, R.L. and J.F. Ely, *Note on the Number Dependence of Nonequilibrium Molecular Dynamics Simulations of Viscosity of Structured Molecules*. J. Chem. Phys., 1992. **96**: 4814-15.
50. Rowley, R.L. and J.F. Ely, *Nonequilibrium molecular-dynamics simulations of structured molecules .2. Isomeric effects on the viscosity of models for normal-hexane, cyclohexane and benzene*. Molecular Physics, 1992. **75**(3): 713-730.
51. Huber, M.L., D.G. Friend, and J.F. Ely, *Prediction of the thermal conductivity of refrigerants and refrigerant mixtures*. Fluid Phase Equil., 1992. **80**: 249-261.
52. Huber, M.L. and J.F. Ely, *An equation of state formulation of the thermodynamic properties of R134a (1,1,1,2-tetrafluoroethane)*. Rev. Int. Froid, 1992. **15**(6): 393-400.
53. Huber, M.L. and J.F. Ely, *Prediction of viscosity of refrigerants and refrigerant mixtures*. Fluid Phase Equil., 1992. **80**: 239-248.
54. Friend, D.G. and J.F. Ely, *Thermodynamics of the methane+ethane system*. Fluid Phase Equilib., 1992. **79**: 77-88.
55. Rowley, R.L. and J.F. Ely, *Nonequilibrium molecular-dynamics simulations of structured molecules .1. Isomeric effects on the viscosity of butanes*. Mol. Phys, 1991. **72**(4): 831-846.
56. Rowley, R.L. and J.F. Ely, *Nonequilibrium molecular dynamics simulations of n-butane and isobutane viscosity*. Mol. Sim., 1991. **7**: 303-323.
57. Friend, D.G., J.F. Ely, and H. Ingham, *Thermophysical properties of ethane*. J. Phys. Chem. Ref. Data, 1991. **20**(2): 275-347.
58. Huber, M.L. and J.F. Ely, *Extension of an improved one-fluid conformal solution theory to real fluid mixtures with large size differences*. Int. J. Thermophys., 1990. **11**(1): 87-96.
59. Ely, J.F., *A predictive, exact shape factor extended corresponding states model for mixtures*. Adv. Cryo. Eng., 1990. **35**: 1511-20.
60. Sherman, G.J., J.W. Magee, and J.F. Ely, *PVT relationships in a carbon dioxide-rich mixture with ethane*. Int. J. Thermophys., 1989. **10**(1): 47-59.
61. McLinden, M.O., et al., *Measurement and Formulation of the Thermodynamic Properties of Refrigerants 134a (1,1,1,2-Tetrafluoroethane) and 123 (1,1-Dichloro-2,2,2-Trifluoroethane)*. ASHRAE Trans.-2, 1989. **95**: 263-83.
62. Hariri, M.H., G.A. Mansoori, and J.F. Ely, *Bioseparations: Design and Engineering of Partitioning Systems*. Bio/Technology, 1989. **7**: 686-88.
63. Friend, D.G., J.F. Ely, and H. Ingham, *Thermophysical properties of methane*. J. Phys. Chem. Ref. Data, 1989. **18**(2): 583-638.
64. Ely, J.F., W.M. Haynes, and B.C. Bain, *Isochoric (p, V(m), T) measurements on CO(2) and on (0.982 CO(2) + 0.018 N(2)) from 250 to 330 K at pressures to 35 MPa*. J. Chem. Thermodyn., 1989. **21**(8): 879-94.
65. Diller, D.E. and J.F. Ely, *Measurements of the Viscosities of Compressed Gaseous Carbon Dioxide, Ethane and Their Mixtures up to 500 K*. High Temperatures- High Pressures, 1989. **21**: 613-20.
66. Magee, J.W. and J.F. Ely, *Isochoric (p, v, T) measurements on CO(2) and (0.98 CO(2) + 0.02 CH(4)) from 225 to 400 K and pressures to 35 MPa*. Int. J. Thermophys., 1988. **9**(4): 547-57.
67. Younglove, B.A. and J.F. Ely, *Thermophysical properties of fluids. II. Methane, ethane, propane, isobutane, and normal butane*. J. Phys. Chem. Ref. Data, 1987. **16**(4): 577-798.
68. Huber, M.L. and J.F. Ely, *Improved conformal solution theory for mixtures with large size ratios*. Fluid Phase Equilib., 1987. **37**: 105-21.
69. Hamad, Z., G.A. Mansoori, and J.F. Ely, *Conformality in the Kirkwood-Buff solution theory of statistical mechanics*. J. Chem. Phys., 1987. **86**(3): 1478-84.
70. Erickson, D.D., T.W. Leland, and J.F. Ely, *A method for improving equations of state near the critical point*. Fluid Phase Equilib., 1987. **37**: 185-205.
71. Chen, L.J., J.F. Ely, and G.A. Mansoori, *Mean density approximation and hard sphere expansion theory: a review*. Fluid Phase Equilib., 1987. **37**: 1-27.
72. Oshmyansky, Y., et al., *The viscosities and densities of selected organic compounds and mixtures of interest in coal liquefaction studies*. Int. J. Thermophys., 1986. **7**(3): 599-608.
73. Magee, J.W. and J.F. Ely, *Specific heats (C(v)) of saturated and compressed liquid and vapor carbon dioxide*. Int. J. Thermophys., 1986. **7**(6): 1163-82.

74. Evans, D.J. and J.F. Ely, *Viscous flow in the stress ensemble*. Mol. Phys., 1986. **59**(5): 1043-8.
75. Ely, J.F., *A test of the mean density approximation for Lennard-Jones mixtures with large size ratios*. Int. J. Thermophys., 1986. **7**(2): 381-93.
76. Bruno, T.J., G.L. Hume, and J.F. Ely, *Hydrogen component fugacities in binary mixtures with methane and propane*. Int. J. Thermophys., 1986. **7**(5): 1033-51.
77. Mansoori, G.A. and J.F. Ely, *Density expansion (DEX) mixing rules: thermodynamic modeling of supercritical extraction*. J. Chem. Phys., 1985. **82**(1): 406-13.
78. Mansoori, G.A. and J.F. Ely, *Erratum: density expansion (DEX) mixing rules: thermodynamic modeling of supercritical extraction [J. Chem. Phys. 82, 406 (1985)]*. J. Chem. Phys., 1985. **83**(3): 1434.
79. Mansoori, G.A. and J.F. Ely, *Statistical mechanical theory of local compositions*. Fluid Phase Equilib., 1985. **22**: 253-75.
80. Baltatu, M.E., et al., *Thermal conductivity of coal-derived liquids and petroleum fractions*. Ind. Eng. Chem., 1985. **Process Des. Dev.**: 24, 325-32.
81. Ely, J.F. and H.J.M. Hanley, *Prediction of transport properties. 2. Thermal conductivity of pure fluids and mixtures*. Ind. Eng. Chem. Fundam., 1983. **22**(1): 90-7.
82. Ely, J.F. and J.K. Baker, *Prediction of the viscosity of pure and mixed cryogenic fluids*. A.I.Ch.E. Symposium Series, 1983. **79**(224): 100-104.
83. Baltatu, M.E., et al., *Thermal conductivity of coal derived liquids*. Proc. Int. Conf. Coal Sci., 1983. **1983**: 757-60.
84. Cullick, A.S. and J.F. Ely, *Densities of vinyl chloride from 5 to 65 degrees C and saturation pressure to 4.2 MPa*. J. Chem. Eng. Data, 1982. **27**: 276-81.
85. Ely, J.F. and H.J.M. Hanley, *Prediction of transport properties. 1. Viscosity of fluids and mixtures*. Ind. Eng. Chem. Fundam., 1981. **20**(4): 323-32.
86. Ely, J.F., *An Enskog correction for size and mass difference effects in mixture viscosity prediction*. J. Res. Natl. Bur. Stand. (U. S.), 1981. **86**(6): 597-604.
87. Ely, J.F. and R. Kobayashi, *Isochoric pressure-volume-temperature measurements for compressed liquid propane*. J. Chem. Eng. Data, 1978. **23**(3): 221-3.
88. Seymour, K., et al., *An Empirical Correlation Among Azeotropic Data*. Ind. Eng. Chem., 1977. **16**(2): 200-7.
89. Holland, P.M., J.F. Ely, and H.J.M. Hanley, *A method for the numerical evaluation of the second virial coefficient for polyatomic molecules*. J. Res. Natl. Bur. Stand. (U. S.), 1977. **82**(2): 123-7.
90. Hanley, H.J.M., J.V. Sengers, and J.F. Ely, *On estimating thermal conductivity coefficients in the critical region of gases*. Therm. Conduct., 1976. **14**: 383-408.
91. Ely, J.F. and H.J.M. Hanley, *The statistical mechanics of non-spherical polyatomic molecules. Application to the properties of carbon dioxide*. Mol. Phys., 1975. **30**(2): 565-78.
92. Ely, J.F. and G.C. Straty, *Dielectric constants and molar polarizabilities of saturated and compressed fluid nitrogen*. J. Chem. Phys., 1974. **61**(4): 1480-5.
93. Ely, J.F. and D.A. McQuarrie, *Calculation of dense fluid transport properties via equilibrium statistical mechanical perturbation theory*. J. Chem. Phys., 1974. **60**(11): 4105-8.
94. Schmoranzler, H., et al., *Observation of the Compton Modified Band for the Scattering of keV Electrons by H₂, He, Ne and Ar*. J. Chem. Phys., 1973. **59**(1): 152-7.
95. Hanley, H.J.M. and J.F. Ely, *The viscosity and thermal conductivity coefficients of dilute nitrogen and oxygen*. J. Phys. Chem. Ref. Data, 1973. **2**(4): 735-55.
96. Ely, J.F., H.J.M. Hanley, and G.C. Straty, *Analysis of the pressure virials and Clausius-Mossotti function for polyatomic gases*. J. Chem. Phys., 1973. **59**(2): 842-8.
97. Ely, J.F. and H.J.M. Hanley, *Analysis of the viscosity and second virial coefficients of non-polar polyatomic gases using the m-6-8 potential*. Mol. Phys., 1972. **24**(3): 683-7.
98. Ely, J.F. and D.A. McQuarrie, *Statistical mechanical theory of electrostriction*. J. Phys. Chem., 1971. **75**(6): 772-775.
99. Ely, J.F. and D.A. McQuarrie, *Quantum corrections to the second dielectric virial coefficient of rare-gas atoms*. J. Chem. Phys., 1971. **54**(7): 2885-8.

Book Chapters

1. Liu, B.; Lusk, M.T. and Ely, J.F.; van Duin; A.C.T.; and Goddard, W.A. III, *Reactive Molecular Dynamics Force Field for the Dissociation of Light Hydrocarbons on Ni(111)*, in *Industrial Application of Molecular Simulations*, M. Meunier, Editor, CRC Press, 2011. p. 231-240.
2. Ely, J.F., *The corresponding states principle*, in *Applied Thermodynamics of Fluids*, A. R. Goodwin, C. Peters and J. V. Sengers, Eds., IUPAC, RSC Publishing, 2010.
3. Kiselev, S.B. and J.F. Ely, *Thermodynamic properties in the critical region*, in *JSRAE Thermodynamic Tables*. 2007. p. 40-44.
4. Ratanapisit, J.R., J.F. Ely, D.J. Isbister, and A. Baranyai, *Thermal conductivity simulation using heat reservoirs*, in *A.I.Ch.E. Symposium Series 325*, P.T. Cummings, P.R. Westmoreland, and B. Carnahan, Editors. 2001. p. 221-225.
5. Ely, J.F. and I.M.F. Marrucho, *The corresponding states principle*, in *Equations of state for fluids and fluid mixtures*, J.V. Sengers, et al., Editors. 2000, Elsevier: Amsterdam. p. 189-230.

Archival Conference Publications

1. Wagg, L., S. Collier, J.D. Way, and J.F. Ely. *The application of a microporous silica membrane to the direct measurement of fugacity in a binary mixture*. in *5th Int. Conf. on Inorganic Membranes*. 1998 p. 168-171.
2. Ely, J.F., W.M. Haynes, C.D. Holcomb, and J.W. Magee. *New Data and Correlations for the Custody Transfer of Natural Gas Liquids*. in *Proc. 74th Gas Processors Association Annual Convention*. 1995: Gas Processors Association, Tulsa, OK p. 35-53.
3. Ely, J.F. and M.L. Huber. *A predictive extended corresponding states model for pure and mixed refrigerants*. in *ASHRAE-Purdue CFC & IRR-Purdue Refrigeration Conf.*, 1990, Purdue University, W. Lafayette, IN p. 383-92.
4. Ely, J.F. and J.W. Magee. *Experimental measurement and prediction of thermophysical property data of carbon dioxide rich mixtures*. in *Proc. 68th Gas Processors Association Annual Convention*. 1989: Gas Processors Association, Tulsa, OK p. 89-98.
5. Ely, J.F. *An equation of state model for pure CO₂ and CO₂ rich mixtures*. in *Proc. 65th Gas Processors Association Annual Convention*. 1986 p. 185-92.
6. Ely, J.F. *Application of the Extended Corresponding States Model to Hydrocarbon Mixtures. (Computer Program EXCST)*. in *Proc. 63rd Gas Processors Association Annual Convention*. 1984: Gas Processors Association, Tulsa, OK p. 9-22.
7. Ely, J.F. and N.A. Olien. *Measurements and data for carbon dioxide in the near critical and supercritical region*. in *Proc. Int. Sch. Hydrocarbon Meas.* 1983 p. 146-9.
8. Ely, J.F. and N.A. Olien. *An overview of fluid thermophysical property research at the National Bureau of Standards*. in *Proc. 62nd Gas Processors Association Annual Convention*. 1983 p. 249-55.
9. Baltatu, M.E., J.F. Ely, M.S. Graboski, H.J.M. Hanley, and R.A.S.E.D. Perkins. *Thermal conductivity of coal derived liquids*. in *Proc. Int. Conf. Coal Sci.* 1983 p. 757-60.
10. Ely, J.F. *Prediction of dense fluid viscosities in hydrocarbon mixtures*. in *Proc. 61st Gas Processors Association Annual Convention*. 1982 p. 9-17.
11. Ely, J.F. and H.J.M. Hanley. *Prediction of the viscosity and thermal conductivity in hydrocarbon mixtures - computer program TRAPP*. in *Proc. 60th Gas Processors Association Annual Convention*. 1981 p. 20-9.
12. Hanley, H.J.M., J.V. Sengers, and J.F. Ely, *On estimating thermal conductivity coefficients in the critical region of gases*. *Therm. Conduct.*, 1976. **14**: 383-408.
13. Carnahan, N.F., G.A. Pope, J.F. Ely, and R.K. Kobayashi. *Ethane Enthalpies - Comparison of Values Derived from Rice P-V-T Studies with Michigan Calorimetric Data*. in *Proc. 54th Annual Gas Processors Association Convention*. 1974 p. 29-30.

Edited Books and Proceedings

1. Ely, J.F., ed. *Proceedings of the Fifteenth Symposium on Thermophysical Properties*. Fluid Phase Equilib. Vol. 222-223. 2004. 343 pp.
2. Ely, J.F., ed. *Proceedings of the Fourteenth Symposium on Thermophysical Properties - Part 1*. Fluid Phase Equilib. Vol. 183-184. 2001. 410 pp.
3. Ely, J.F., ed. *Proceedings of the Fourteenth Symposium on Thermophysical Properties - Part 2*. Fluid Phase Equilib. Vol. 185. 2001. 418 pp.
4. Ely, J.F. and W.M. Haynes, eds. *Proceedings of the Thirteenth Symposium on Thermophysical Properties*. Fluid Phase Equilib. Vol. 150-151. 1998. 849 pp.
5. Ely, J.F., ed. *Proceedings of the Seventh International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design - Part 1*. Fluid Phase Equilib. Vol. 116. 1996. 544 pp.
6. Ely, J.F., ed. *Proceedings of the Seventh International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design - Part 2*. Fluid Phase Equilib. Vol. 117. 1996. 393 pp.
7. Ely, J.F., ed. *Proceedings of the 11th Symposium on Thermophysical Properties - Part 1*. Fluid Phase Equilib. Vol. 75. 1992. 297 pp.
8. Ely, J.F., ed. *Proceedings of the 11th Symposium on Thermophysical Properties - Part 2*. Fluid Phase Equilib. Vol. 76. 1992. 295 pp.
9. Ely, J.F., ed. *Proceedings of the 11th Symposium on Thermophysical Properties - Part 3*. Fluid Phase Equilib. Vol. 79. 1992. 326 pp.
10. Ely, J.F., ed. *Proceedings of the 11th Symposium on Thermophysical Properties - Part 4*. Fluid Phase Equilib. Vol. 80. 1992. 331 pp.
11. Ely, J.F., ed. *Proceedings of the 11th Symposium on Thermophysical Properties - Part 5*. Fluid Phase Equilib. Vol. 88. 1993. 303 pp.
12. Bruno, T.J. and J.F. Ely, eds. *Supercritical Fluid Technology: Reviews in Modern Theory and Applications*. 1991: CRC Press.

Archival Peer-Reviewed Technical Reports

1. Ely, J.F., *Volume Correction Factors for Natural Gas Liquid-Phase II*. Gas Processors Association Research Report 148, 1996
2. Howley, J.A., J.W. Magee, and J.F. Ely, *A Predictive Model for the Thermophysical Properties of Carbon Dioxide Rich Mixtures*, Gas Processors Association Research Report 136, 1993
3. Friend, D.G., H. Ingham, and J.F. Ely, *Tables for the thermophysical properties of ethane*, National Institute of Standards and Technology Technical Note 1443, 1991
4. Ely, J.F., *Volume correction factors for natural gas liquids*, Gas Processors Association Research Report 134, 1991
5. Huber, M.L. and J.F. Ely, *Properties of Lennard-Jones Mixtures at Various Temperatures and Energy Ratios with a Size Ratio of Two*, National Institute of Standards and Technology Technical Note 1331, 1989
6. Friend, D.G., H. Ingham, and J.F. Ely, *Tables for the thermophysical properties of methane*, National Institute of Standards and Technology Technical Note 1325, 1989
7. Ely, J.F. and J.K. Baker, *A review of supercritical fluid extraction*, U.S. National Bureau of Standards Technical Note 1071, 1983
8. Eaton, B.E., J.F. Ely, H.J.M. Hanley, R.D. McCarty, and J.C. Rainwater, *Phase equilibria: An informal symposium*, U.S. National Bureau of Standards Technical Note 1061, 1983
9. Ely, J.F. and H.J.M. Hanley, *A computer program for the prediction of viscosity and thermal conductivity in hydrocarbon mixtures*, U. S. National Bureau of Standards Technical Note 1039, 1981