

J. Richard Elliott
Department of Chemical Engineering
The University of Akron
(330) 972-7253
elliott1@uakron.edu

MAJOR TEXTS

'Introductory Chemical Engineering Thermodynamics,' J. Richard Elliott and Carl T. Lira, Prentice-Hall, 660 pp., 1999. Online at: <http://www.egr.msu.edu/~lira/thermtxt.htm>

'Introductory Chemical Engineering Thermodynamics, 2ed,' J. Richard Elliott and Carl T. Lira, Prentice-Hall, 869 pp., 2012. Online at: <http://chethermo.net>

PUBLICATIONS IN ARCHIVAL JOURNALS

1. Combined temperature and density series for fluid-phase properties. I. Square-well spheres, J. Richard Elliott, Andrew J. Schultz, David A Kofke, *J. Chem. Phys.*, 143:114110 (2015).
2. A simple extrapolation of thermodynamic perturbation theory to infinite order, Ahmad F. Ghobadi, J. Richard Elliott, *J. Chem. Phys.*, 143:114107 (2015).
3. Adapting SAFT- γ Perturbation Theory To Site-Based Molecular Dynamics Simulation: 3. Molecules with partial charges at bulk phases, confined geometries and interfaces, Ahmad F. Ghobadi, J. Richard Elliott, *J. Chem. Phys.*, 141:094708 (2014).
4. Adapting SAFT- γ Perturbation Theory To Site-Based Molecular Dynamics Simulation: 2. Confined Fluids and Vapor-Liquid Interfaces, Ahmad F. Ghobadi, J. Richard Elliott, *J. Chem. Phys.*, 141:024708 (2014).
5. Transferable Intermolecular Potential Models for a Broad Range of Organic Compounds, Amanda D. Sans, Amir Vahid, J. Richard Elliott, *J. Chem. Eng. Data*, 59:3069-3079 (2014).
6. The Athermal Contribution to the Entropy of Mixing, Amir Vahid, Neil H. Gray, and J. Richard Elliott, *Macromolecules*, 47:1514-1531 (2014).
7. Adapting SAFT- γ Perturbation Theory To Site-Based Molecular Dynamics Simulation: 1. Homogeneous Fluids, Ahmad F. Ghobadi, J. Richard Elliott, *J. Chem. Phys.*, 139:234104 (2013).
8. Renormalization Group Adaptation To Equations Of State From Molecular Simulation. Ahmad F. Ghobadi, J. Richard Elliott, *Ind. Eng. Chem. Res.*, 52:7030-7043 (2013).
9. Polymer Equations of State Derived From Molecular Simulation, Amir Vahid and J. Richard Elliott, *Fluid Phase Equilibria*, 351:61-68 (2013).

10. Application of the Step Potential for Equilibria and Dynamics (SPEAD) Method to Bioderived Esters and Acetals, Abu M. Hassan, Dung T. Vu, Damien A. Bernard-Brunel, J. Richard Elliott, Dennis J. Miller, Carl T. Lira, *Ind. Eng. Chem. Res.*, 51: 3209-3214 (2012).
11. Optimization Of Transferable Site-Site Potentials Using A Combination Of Stochastic And Gradient Search Algorithms, Sinan Ucyigitler, Mehmet C. Camurdan, J. Richard Elliott, *Ind. Eng. Chem. Res.*, 51: 6219-6231 (2012).
12. Investigation on the solubility of SO₂ and CO₂ in imidazolium based ionic liquids using NPT Monte Carlo simulation, Ahmad F. Ghobadi, Vahid Taghikhani, J. Richard Elliott, *JPCB*, 115:13599-13607 (2011).
13. Evaluating Perturbation Contributions in SAFT Models by Comparing to Molecular Simulation of N-Alkanes, Ahmad F. Ghobadi, J. Richard Elliott, *Fluid Phase Equilibria*, 305:57-66 (2011).
14. 'Historical Perspective and Current Outlook for Molecular Dynamics As a Chemical Engineering Tool,' Edward J. Maginn and J. Richard Elliott, *Ind. Eng. Chem. Res.*, 49:3059-3078 (2010).
15. 'Self-Diffusivity Estimation By Molecular Dynamics,' Z. Nevin Gerek and J. Richard Elliott, *Ind. Eng. Chem. Res.*, 49:3411-3423 (2010).
16. 'A Survey of the Role of Thermodynamics and Transport Properties in CHE University Education in Europe and the USA,' P. Ahlström, K. Aim, R. Dohrn, J.R. Elliott, G. Jackson, J.N. Jaubert, E.A. Macedo, J.P.-Pokki, K. Reczey, A. Victorov, L.F. Žilnik, I.G. Economou, *Chem. Eng. Ed.*, 44(1):35-43 (2010).
17. 'A Simple Explanation of Complexation,' J. Richard Elliott, *Chem. Eng. Ed.*, 44(1):13-22 (2010).
18. 'Transferable Intermolecular Potentials and Equations of State for Carboxylic Acids and Their Phase Behavior,' Amir Vahid, J. Richard Elliott, *AIChE J.*, 56:485-505 (2010).
19. 'Finitely Limited Group Contribution Correlations for Boiling Temperatures,' Fateme Sadat Emami, Amir Vahid, J. Richard Elliott, Farzaneh Feyzi, *J. Chem. Thermo.*, 31:530-537 (2009).
20. 'Correlation Of Mixture Vapor-Liquid Equilibria With The SPEADM Model,' Amir Vahid, Amanda D. Sans, J. Richard Elliott, *Ind. Eng. Chem. Res.*, 47:7955-7964 (2008).
<http://pubs.acs.org/cgi-bin/download.pl?ie800374h/L6Za>

21. 'Group Contribution Prediction of Vapor Pressure with SAFT, PC-SAFT and ESD Equations of State,' Fateme Sadat Emami, Amir Vahid, J. Richard Elliott, Farzaneh Feyzi, *Ind. Eng. Chem. Res.*, 47:8401–8411 (2008). <http://pubs.acs.org/cgi-bin/download.pl?ie800329r/A7on>
22. 'Inferring Transferable Potential Models,' Sinan Ucyigitler, Mehmet C. Camurdan, Metin Turkay, J. Richard Elliott, *Molecular Simulation.*, 34:147-154 (2008).
23. 'Butadiene Purification Using Polar Solvents. Analysis of Mixture Nonideality Using Data and Estimation Methods,' Paul M. Mathias, J. Richard Elliott, Andreas Klamt, *Ind. Eng. Chem. Res.*, 47:4996–5004 (2008).
24. 'Transferable Potentials for Perfluorinated Molecules,' Amanda D. Sans, J. Richard Elliott, *Fluid Phase Equilibria*, 263:182-189 (2008).
25. 'Combining Molecular Dynamics and Chemical Process Simulation: The SPEADMD Model' *AsiaPacific J. Chem. Eng.*, 2:257-271 (2007).
26. 'Transferable Potentials for Alcohol-Amine Interactions,' J. Richard Elliott, Amir Vahid, Amanda D. Sans, *Fluid Phase Equilibria*, 256:4-13 (2007).
27. 'Molecular dynamic simulations and global equation of state of square-well fluids with well-widths from 1.1 to 2.1,' Sergei B. Kiselev, James F. Ely, J. Richard Elliott, *Mol. Phys.*, 104:2545-2559 (2006).
28. 'Asymptotic Trends in Thermodynamic Perturbation Theory,' J. Richard Elliott and Neil H. Gray, *J. Chem. Phys.*, 123:184902 (2005).
29. 'Transferable Step Potentials for Amines, Amides, Acetates, and Ketones,' Suhan Baskaya, Neil Gray, Z. Nevin Gerek, and J. Richard Elliott, *Fluid Phase Equilibria*, 236:42-52 (2005).
30. 'Molecular Modeling of Isomer Effects in Naphthenic and Aromatic Hydrocarbons,' Neil Gray, Z. Nevin Gerek, and J. Richard Elliott, *Fluid Phase Equilibria*, 228-229C, 147-153 (2005).
31. 'Gas Permeation in the Silicalite Single Crystal Membrane,' M.G. Ahunbay, J.R. Elliott, Jr., and O. Talu, *Adsorption*, 11(sup1):313-318 (2005).
32. 'The Effect of Surface Resistances on the Diffusion of Binary Mixtures in the Silicalite Single Crystal Membrane,' M.G. Ahunbay, J.R. Elliott, Jr., and O. Talu, *J. Phys. Chem. B*, 109:923-929 (2005).
33. 'Surface Resistance to Permeation Through the Silicalite Single Crystal Membrane: Variation with Permeant,' M.G. Ahunbay, J.R. Elliott, and O. Talu, *J. Phys. Chem. B*, 108:7801-7808 (2004).

34. 'Transferable Step Potentials for the Straight Chain Alkanes, Alkenes, Alkynes, Ethers, and Alcohols,' Ozlem Unlu, Neil Gray, Z. Nevin Gerek, and J. Richard Elliott, *Ind. Eng. Chem. Res.*, 43:1788-1793 (2004).
35. 'Binary Interactions of Poly(Ethylene Covinyl Alcohol) with Poly(4-Vinyl Pyridine) and Poly(*n*-Butyl Methacrylate),' S. Keskin and J.R. Elliott, *Ind. Eng. Chem. Res.*, 42:6331 (2003).
36. 'The Diffusion Processs of Methane in the Silicalite Single Crystal Membrane,' M.G. Ahunbay, J.R. Elliott, Jr., and O. Talu, *J. Phys. Chem. B*, 106:5163 (2002).
37. 'Phase Diagrams for Multi-step Potential Models of *n*-Alkanes by DMD/TPT,' J. Cui and J.R. Elliott, Jr., *J. Chem. Phys.*, 116:8625 (2002).
38. 'Computer Simulations and Crossover Equation of State of Square-Well Fluids,' S.B. Kiselev, J.F. Ely, L. Lue, and J.R. Elliott, Jr., *Fluid Phase Equilibria*, 200:121 (2002).
39. 'Extension of the ESD Equation to Polymer Solutions,' J.R. Elliott, Jr., R.N. Natarajan, *Ind. Eng. Chem. Res.* 41:1043 (2002).
40. 'Optimized Step Potential Models for *n*-Alkanes and Benzene,' J.R. Elliott, Jr., *Fluid Phase Equilibria*, 194:161 (2002).
41. 'High-Pressure Vapor-Liquid Equilibrium for Dimethyl Ether + Isopropanol and Dimethyl Ether + Isopropanol + Water,' M.M. Elbaccouch, J.R. Elliott, Jr., *J. Chem. Eng. Data*, 46:675 (2001). DOI: 10.1021/je000317e
42. 'Phase Envelopes For Variable Width Square Well Chain Fluids,' J. Cui and J.R. Elliott, Jr., *J. Chem. Phys.*, 114:7283 (2001).
43. 'The Bancroft Point and Vapor-Liquid Equilibria in the System Isopropanol + Benzene,' J.R. Elliott, Jr., J.C. Rainwater, *Fluid Phase Equilibria*, 175:229 (2000). Database at: <http://130.101.3.26/~chem/fclty/elliott/BancroftPts.zip>
44. 'High-Pressure Vapor-Liquid Equilibrium for Dimethyl Ether + Ethanol and Dimethyl Ether + Ethanol + Water,' M.M. Elbaccouch, J.R. Elliott, Jr., *J. Chem. Eng. Data*, 45:1080 (2000).
45. 'Critical Compressibility Factors for Chain Molecules,' L. Lue, D.G. Friend, J.R. Elliott, Jr., *Molecular Physics*, 98:1473-1477 (2000).
46. Vapor-Liquid Equilibria for an R134a/Lubricant Mixture: Measurements and Equation-of-State Modeling,' Marcia L. Huber, Cynthia D. Holcomb, Stephanie L. Outcalt, J. Richard Elliott, Jr., *ASHRAE Transactions: Symposia*, 106(1):768 (2000).

47. 'High-Pressure Vapor Liquid Equilibria of R-22 + Ethanol and R-22 + Ethanol + Water,' M.M. Elbaccouch, M.B. Raymond, J.R. Elliott, Jr., *J. Chem. Eng. Data*, 45:280 (2000).
48. 'Vapor Liquid Equilibria of Square-Well Chains,' L. Hu, H. Rangwalla, J. Cui, J.R. Elliott, Jr., *J. Chem. Phys.*, 111:1293 (1999).
49. 'Vapor Liquid Equilibria of Square-Well Spheres,' J.R. Elliott, Jr. and L. Hu, *J. Chem. Phys.*, 110:3043 (1999).
50. 'Chemical Vapor Deposition of Carbon on Graphite by Methane Pyrolysis', S. Bammidipati, G.D. Stewart, J.R. Elliott, Jr., S.A. Gokoglu, M.J. Purdy, *AIChE J.*, 42:3123 (1996).
51. 'Screening Effects on Hydrogen Bonding in Chain Molecular Fluids: Thermodynamics and Kinetics', J-X. Liu, J.R. Elliott, Jr., *Ind. Eng. Chem. Res.* 35:2369 (1996).
52. 'Efficient Implementation of Wertheim's Theory for Multicomponent Mixtures of Multiply Associating Species', J.R. Elliott, Jr., *Ind. Eng. Chem. Res.* 35:1624 (1996).
53. 'Chemical Engineering Education in Turkey and the United States', J.R. Elliott, Jr., *Chemical Engineering Education*, 30:150 (1996).
Online at: <http://130.101.3.26/~chem/fclty/elliott/FulbRep.pdf>
54. 'Screening vs. Hydrogen Bonding in the Poly(vinylpyridine)+Poly(vinylbutyral) System', M.L. Franzen, J.R. Elliott, Jr., Kyu, T., *Macromolecules*, 28:5147 (1995)
55. 'Theory and Measurement of Fates of H₂S Scavengers', J.R. Elliott, Jr., M.B. Raymond, B. Kalpakci, N.F. Magri, *Soc. Pet. Eng., SPE*:28949 (1995)
56. 'Discontinuous molecular dynamics simulation of hydrogen bonding systems', J.-X. Liu, T.L. Bowman, II, and J.R. Elliott, Jr., *Ind. Eng. Chem. Res.*, 33:957 (1994).
57. 'Correlation and prediction of binary VLE in systems containing gases, hydrocarbons, alcohols, and water,' A.S. Puhala and J.R. Elliott, Jr., *Ind. Eng. Chem. Res.* 32:3174 (1993).
58. 'Intramolecular variations in structure of chain molecular fluid mixtures', V.J. Vasudevan and J.R. Elliott, Jr., *Fluid Phase Equilibria*, 83:33 (1993).
59. 'Fluid Structure for Sophomores', J. Richard Elliott, Jr., *Chem. Eng. Ed.*, 27:44 (1993).
60. 'Multiphase equilibrium analyses of complex mixtures via an association-based equation of state', S.J. Suresh and J.R. Elliott, Jr., *Ind. Eng. Chem. Res.*, 31:2783 (1992).
61. 'Microcellular foams via polymerization in near-critical diluents', G. Srinivasan and J.R. Elliott, Jr., *Ind. Eng. Chem. Res.*, 31:1414 (1992).

62. 'Structure and thermodynamics of chain molecular fluid mixtures', V.J. Vasudevan and J.R. Elliott, Jr., *Molecular Physics*, 75:443 (1992).
63. 'Microcellular methacrylates: Effect of supercritical drying on pore size and density', J.R. Elliott, Jr., R. Akhaury, and G. Srinivasan, *Polymer Communications*, 32(1):11 (1991).
64. 'Binary and multicomponent vapor-liquid equilibria of synthesis gas components, methanol, and water with tetraethylene glycol dimethyl ether' P. Khosla, C. Krishnan, J.R. Elliott, Jr., and J.M. Berty, *Chem. Eng. Comm.*, 102:35 (1991).
65. 'Simulation of a three-phase reactor for the solvent methanol process', C. Krishnan, J.R. Elliott, Jr., and J.M. Berty, *Chem. Eng. Comm.*, 105:155 (1991).
66. 'Applications of a generalized equation of state for associating mixtures', J.R. Elliott, Jr. and S.J. Suresh, *Ind. Eng. Chem. Res.*, 30:523 (1991).
67. 'Continuous operation of the Berty reactor for the Solvent Methanol Process', C. Krishnan, J.R. Elliott, Jr., and J.M. Berty, *Ind. Eng. Chem. Res.*, 30:1413 (1991).
68. 'A simple equation of state for non-spherical and associating molecules', J.R. Elliott, Jr., S.J. Suresh, and M.D. Donohue, *Ind. Eng. Chem. Res.*, 29:1476 (1990).
69. 'Beat the Equilibrium', J.M. Berty, C. Krishnan, and J.R. Elliott, Jr., *ChemTech*, 20:624 (1990).
70. 'Attractive force effects in chain molecular fluids', J.R. Elliott, Jr., U.S. Kanetkar, and V.J. Vasudevan, *Molecular Physics*, 71:883 (1990).
71. 'Theory and simulation of chain molecule fluid structure', J.R. Elliott, Jr. and U.S. Kanetkar, *Molecular Physics*, 71:871 (1990).
72. 'Evaluation of the equation of state method for calculation of the critical properties of mixtures', J.R. Elliott, Jr. and T.E. Daubert, *Ind. Eng. Chem. Res.*, 26:1686-1691 (1987).
73. 'The temperature dependence of the hard sphere diameter', J.R. Elliott, Jr. and T.E. Daubert, *Fluid Phase Equilibria*, 31:153-160 (1986). $d_{hs}/r_{min} = [n(0.0093n-0.0592)/\beta\epsilon^2+(n-1)/\beta\epsilon+1]^{-1/(2n+1)}$
74. 'Revised procedures for phase equilibrium calculations with the Soave equation of state', J.R. Elliott, Jr. and T.E. Daubert, *I&EC Proc. Des. Dev.*, 24:743 (1985).'

PUBLICATIONS IN REFEREED BOOKS

'Critical Phase Behavior,' J.R. Elliott, *Encyclopedia of Chemical Engineering.*, Sunggyu Lee, Ed. Marcel Dekker (2006).

'The Soave Equation,' J.R. Elliott, *Encyclopedia of Chemical Engineering.*, Sunggyu Lee, Ed. Marcel Dekker (2006).

'Hydrogen Bonding,' J.R. Elliott, *Encyclopedia of Chemical Engineering.*, Sunggyu Lee, Ed. Marcel Dekker (2006).

'Multi-Step Potential Modeling of Methane by DMD/TPT,' J.R. Elliott, Jr., J. Cui, *AIChE Symp. Ser.*, 325:159 (2001).

'Light Scattering Study of Polymer Network Formation in a Supercritical Diluent', J.R. Elliott, Jr. and H.M. Cheung, *ACS Symp. Ser.*, 514:271 (1993).

'Critical Properties,' Chapter 4 in Technical Data Book, T.E. Daubert and R.P. Danner (eds.), American Petroleum Institute, Washington (1988).

PATENTS

'Microcellular Foams', Elliott, Jr., J.R., Srinivasan, G., Dhanuka, M., Akhaury, R., U.S. Patent# 5128382, Issued July, 7, 1992.

'Microcellular Foams: Compositions of Matter', Elliott, Jr., J.R., Srinivasan, G., Dhanuka, M., Akhaury, R., U.S. Patent, 5,252,620, Issued October 12, 1993.