

## 2009

1. I. Tsivintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Solid – Liquid Equilibrium in Pharmaceutical – Solvent Mixtures: Systems with Complex Hydrogen Bonding Behavior", AIChE J., 55(3), 756 - 770 (2009).

[Follow this link to the full paper.](#)

2. T. Spyriouni, G.C. Boulougouris and D.N. Theodorou, "Prediction of Sorption of CO<sub>2</sub> in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme", Macromolecules, 42(5), 1759 - 1769 (2009).

[Follow this link to the full paper.](#)

3. I. Tsivintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents", J. Phys. Chem. B, 113(18), 6446 - 6458 (2009).

[Follow this link to the full paper.](#)

4. G.E. Logotheti, J. Ramos, I.G. Economou, "Molecular Modeling of Imidazolium - Based [Tf

2  
N

-  
] Ionic Liquids: Microscopic  
Structure, Thermodynamic and Dynamic Properties and Segmental Dynamics  
”  
,  
J. Phys. Chem. B, 113(20), 7211 - 7224 (2009).

[Follow this link to the full paper.](#)

5. M. Yiannourakou, I.G. Economou and I.A. Bitsanis, “Phase Equilibrium of Colloidal Suspensions with Particle Size Dispersity: A Monte Carlo Study”, J. Chem. Phys., 130(19), 194902-1 - 194902-10 (2009).

[Follow this link to the full paper.](#)

6. N.M. Garrido, A.J. Queimada, M. Jorge, E.A. Macedo and I.G. Economou, "1-Octanol / Water Partition Coefficient of n-Alkanes from Molecular Simulations of Absolute Solvation Free Energies", J. Chem. Theory Comput., 5(9), 2436 - 2446 (2009).

[Follow this link to the full paper.](#)

7. M. Yiannourakou, L. Marsela, F. de Meyer and B. Smit, “Towards an Understanding of Membrane-Mediated Protein-Protein Interactions”, Faraday Discuss, in press (2009)

[Follow this link to the full paper.](#)

## 2008

1. Z. Kechagia, C. Kiparissides and I.G. Economou, "Determination of Liquid – Gas Partition Coefficients of BuA and MMA by Headspace-Gas Chromatography Utilizing the Phase Ratio Variation Method", Fluid Phase Equil., 266, 21 – 30 (2008).

[Follow this link to the full paper.](#)

2. I.G. Economou, E.K. Karakatsani, G.-E. Logotheti, J. Ramos and A. Vanin, "Multi-scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-Based Ionic Liquids: Ab initio DFT Calculations, Molecular Simulation and Equation of State Predictions", Oil & Gas Sci. Tech., 63(3), 283 – 293 (2008).

[Follow this link to the full paper.](#)

3. A. Grenner, I. Tsvintzelis, G.M. Kontogeorgis, I.G. Economou and C. Panayiotou, "Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the simplified Perturbed Chain-Statistical Associating Fluid Theory (sPC-SAFT). I. Vapor – Liquid Equilibria", Ind. Eng. Chem. Res., 47(15), 5636 – 5650 (2008).

[Follow this link to the full paper.](#)

4. I. Tsvintzelis, A. Grenner, I.G. Economou and G.M. Kontogeorgis, "Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the simplified Perturbed Chain-Statistical Associating Fluid Theory (sPC-SAFT). II. Liquid – Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems", Ind. Eng. Chem. Res., 47(15), 5651 – 5659 (2008).

[Follow this link to the full paper.](#)

5. Z.A. Makrodimitri and I.G. Economou, “Atomistic Simulation of Poly(dimethylsiloxane) Permeability Properties to Gases and n-Alkanes”, *Macromolecules*, 41(15), 5899 – 5907 (2008).

[Follow this link to the full paper.](#)

6. G. Tsolou, V.G. Mavrantzas, Z.A. Makrodimitri, I.G. Economou and R. Gani, “Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene”, *Macromolecules*, 41(16), 6228 – 6238 (2008).

[Follow this link to the full paper.](#)

7. E.K. Karakatsani, I.G. Economou, M.C. Kroon, M.D. Bermejo, C.J. Peters and G.-J. Witkamp, “Equation of State Modeling of the Phase Equilibria of Ionic Liquid Mixtures at Low and High Pressure”, *Phys. Chem. Chem. Phys.*, 10(40), 6160 – 6168 (2008).

[Follow this link to the full paper.](#)

## **2007**

1. Z.A. Makrodimitri, R. Dohrn and I.G. Economou, “Atomistic Simulation of Poly(dimethylsiloxane): Force Field Development, Structure and Thermodynamic Properties of Polymer Melt and Solubility of n-Alkanes, n-Perfluoroalkanes, Noble and Light Gases”, *Macromolecules*, 40(5), 1720 – 1729 (2007).

[Follow this link to the full paper.](#)

2. Tsivintzelis, T. Spyriouni and I.G. Economou, “Modeling of Fluid Phase Equilibria with Two Thermodynamic Theories: Non-Random Hydrogen Bonding (NRHB) and Statistical Associating Fluid Theory (SAFT)”, *Fluid Phase Equil.*, 253, 19 – 28 (2007).

[Follow this link to the full paper.](#)

3. C. Panayiotou, I. Tsvintzelis and I.G. Economou, "Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 2. Multicomponent Mixtures", *Ind. Eng. Chem. Res.*, 46(8), 2628 - 2636 (2007).

[Follow this link to the full paper.](#)

4. L.D. Peristeras, A.N. Rissanou, I.G. Economou and D.N. Theodorou, "Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends", *Macromolecules*, 40(8), 2904 - 2914 (2007).

[Follow this link to the full paper.](#)

5. A.N. Rissanou, M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Amorphous and Crystalline States of Ultrasoft Colloids: A Molecular Dynamics Study", *Rheol. Acta*, 46(5), 755 - 764 (2007).

[Follow this link to the full paper.](#)

6. A.N. Rissanou, L.D. Peristeras and I.G. Economou, "Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear - Tri-arm Polyethylene Blends from Monte Carlo Simulation", *Polymer*, 48(13), 3883 - 3892 (2007).

[Follow this link to the full paper.](#)

7. I.G. Economou, Z.A. Makrodimitri, G.M. Kontogeorgis and A. Tihic, "Solubility of Gases and Solvents in Silicon Polymers: Molecular Simulation and Equation of State Modeling", *Molec. Simul.*, 33(9 - 10) 851 - 860 (2007).

[Follow this link to the full paper.](#)

8. E.K. Karakatsani, I.G. Economou, M.C. Kroon, C.J. Peters and G.-J. Witkamp, "tPC-PSAFT Modeling of Gas Solubility in Imidazolium-Based Ionic Liquids", *J. Phys. Chem. C*, 111(43), 15487 - 15492 (2007).

[Follow this link to the full paper.](#)

9. T. Spyriouni, C. Tzoumanekas, D. Theodorou, F. Muller-Plathe, G. Milano, "Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts: Structure, Thermodynamic Properties, Chain Conformation, and Entanglements", *Macromolecules*, 40(10), 3876 - 3885 (2007).  
[Follow this link to the full paper.](#)

## 2006

1. A.N. Rissanou, M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Temperature Induced Crystallization in Concentrated Suspensions of Multi-Arm Star Polymers: A Molecular Dynamics Study", *J. Chem. Phys.*, 124(4), 044905-1 – 044905-11 (2006).

2. E.K. Karakatsani and I.G. Economou, "Perturbed Chain-Statistical Associating Fluid Theory Extended to Dipolar and Quadrupolar Molecular Fluids", *J. Phys. Chem. B*, 110(18), 9252 – 9261 (2006).

3. M.C. Kroon, E.K. Karakatsani, I.G. Economou, G.-J. Witkamp and C.J. Peters, "Modeling of the Carbon Dioxide Solubility in Imidazolium-Based Ionic Liquids with the tPC-PSAFT Equation of State", *J. Phys. Chem. B*, 110(18), 9262 – 9269 (2006).

4. E.K. Karakatsani, G.M. Kontogeorgis and I.G. Economou, "Evaluation of the Truncated Perturbed Chain – Polar Statistical Associating Fluid Theory for Complex Mixture Fluid Phase Equilibria", *Ind. Eng. Chem. Res.*, 45(17), 6063 – 6074 (2006).

5. Z.A. Makrodimitri, V.E. Raptis and I.G. Economou, "Molecular Dynamics Simulation of Structure, Thermodynamic and Dynamic Properties of Poly(dimethylsilamethylene), Poly(dimethylsilatri-methylene) and their Alternating Copolymer", *J. Phys. Chem. B*, 110(32), 16047 – 16058 (2006).

6. A.N. Rissanou, I.G. Economou and A.Z. Panagiotopoulos, "Monte Carlo Simulation of the Phase Behavior of Model Dendrimers", *Macromolecules*, 39(18), 6298 – 6305 (2006).

7. E.A. Tritopoulou and I.G. Economou, "Molecular Simulation of Structure and Thermodynamic Properties of Pure Tri- and Tetra-Ethylene Glycols and Their Aqueous Mixtures", *Fluid Phase Equil.*, 248(2), 134 – 146 (2006).

8. I.A. Bitsanis, A.N. Rissanou, M. Yiannourakou, I.G. Economou and D. Vlassopoulos, "Mesoscopic Simulations of T-Induced Solidification in Dense Suspensions of Ultrasoft Supramolecules", *Lecture Series on Comp. and Comput. Sci.*, 6, 1 – 4 (2006).

## **2005**

1. L. Peristeras, I.G. Economou and D.N. Theodorou, "Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves" *Macromolecules*, 38(2), 386 - 397 (2005).

2. I.G. Economou, V.E. Raptis, V.S. Melissas, D.N. Theodorou, J. Petrou and J. Petropoulos, "Molecular Simulation of Structure, Thermodynamic and Transport Properties of Polymeric Membrane Materials for Hydrocarbon Separation" *Fluid Phase Equil.*, 228-229, 15 - 20 (2005).

3. M. Makowska-Janusik, H. Reis, M.G. Papadopoulos and I.G. Economou, "Peculiarities of Electric Field Alignment of Non-Linear Optical (NLO) Chromophores Incorporated Into Thin Film Polymer Matrix" *Theor. Chem. Acc.*, 114(1), 153-158 (2005).

4. E.K. Karakatsani, T. Spyriouni and I.G. Economou, "Extended SAFT Equations of State for Dipolar Fluids" *AIChE J.*, 51(8), 2328 - 2342 (2005).

5. T. Spyriouni and I.G. Economou,  
"Evaluation of SAFT and PC-SAFT Models for the Description of Homo- and Co-Polymer Solution Phase Equilibria"  
Polymer, 46(24), 10772 - 10781 (2005).

6. N. Zacharopoulos, N. Vergadou and D.N. Theodorou ,  
"Coarse-graining using pre-tabulated potentials: Liquid benzene"  
J. Chem. Phys., 122, 244111 (2005).

## **2004**

1. T. Lindvig, I.G. Economou, R.P. Danner, M.L. Michelsen and G.M. Kontogeorgis,  
"Modelling of Multicomponent Vapor-Liquid Equilibria for Polymer-Solvent Systems"  
Fluid Phase Equil., 220(1), 11-20 (2004).

2. M. Makowska-Janusik, H. Reis, M.G. Papadopoulos, I.G. Economou and N. Zacharopoulos,  
"Molecular Dynamics Simulations of Electric Field Poled Nonlinear Optical Chromophores Incorporated in a Polymer Matrix"  
J. Phys. Chem. B., 108(2), 588-596 (2004).

3. V.E. Raptis, I.G. Economou, D.N. Theodorou, J. Petrou and J.H. Petropoulos,  
"Molecular Dynamics Simulation of Structure and Thermodynamic Properties of Poly(dimethylsilamethylene) and Hydrocarbon Solubility Therein: Towards the



Development of Novel Membrane Materials for Hydrocarbon Separation"  
Macromolecules, 37(3), 1102-1112 (2004).

4. C. Panayiotou, M. Pantoula, E. Stefanis, I. Tsivintzelis and I.G. Economou,  
"Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 1. Pure  
Fluids"  
Ind. Eng. Chem. Res., 43(20), 6592-6606 (2004).

5. A. Alentiev, I.G. Economou, E. Finkelshtein, J. Petrou, V.E. Raptis, M.  
Sanopoulou, S. Soloviev, N. Ushakov and Y. Yampolski i,  
"Transport Properties of Silmethylene Homo-polymers and Random Copolymers:  
Experimental Measurements and Molecular Simulation"  
Polymer, 45(20), 6933-6944 (2004).

6. G.K. Papadopoulos, G.K., H. Jobic, D.N. Theodorou,  
"Transport diffusivity of N<sub>2</sub> and CO<sub>2</sub> in silicalite: Coherent quasielastic neutron  
scattering neasurements and molecular dynamics simulations"  
J. Phys. Chem. B, 108, 12948-12756 (2004).

## **2003**

1. A. Oke, H. Mahgerefteh, I. Economou and Y. Rykov,  
"A Transient Outflow Model for Pipeline Puncture"Chem. Eng. Sci., 58(20),  
4591-4604 (2003).

2. E.A. Tritopoulou, G.D. Pappa, E.C. Voutsas, I.G. Economou and D.P.  
Tassios,  
"Modeling of Liquid-Liquid Phase Equilibria in Aqueous Solutions of Poly(ethylene  
glycol) with a UNIFAC-Based Model"

Ind. Eng. Chem. Res., 42(21), 5399-5408 (2003).

## 2002

1. S.A. Soloviev, Yu.P. Yampolskii, I.G. Economou, N.V. Ushakov and E.Sh. Finkelshtein,  
"Thermodynamic Parameters of Hydrocarbon Sorption by Poly(silimethylenes)", Pol. Sci. A, 44(3), 293 - 300 (2002).
2. I.G. Economou, "Statistical Associating Fluid Theory: A Successful Model for the Calculation of Thermodynamic and Phase Equilibrium Properties of Complex Fluid Mixtures", Ind. Eng. Chem. Res., 41(5), 953 - 962 (2002).
3. N. Zacharopoulos and I.G. Economou, "Morphology and Organization of Poly(propylene imine) Dendrimers in the Melt from Molecular Dynamics Simulation",  
Macromolecules, 35(5), 1814 - 1821 (2002).
4. Makrodimitris, K.; Papadopoulos, G.K.; Philippopoulos, C.; Theodorou, D.N.,  
"Parallel tempering method for reconstructing isotropic and anisotropic porous media",  
J. Chem. Phys., 117, 5876-5884 (2002).
5. Rabias, I.; Langlois, C.; Provata, A.; Howlin, B.J.; Theodorou, D.N.,  
"Linking the atomistic scale and the mesoscale: molecular orbital and solid state packing calculations on poly(p-phenylene)",  
Polymer, 43, 185-193 (2002).

## 2001

1. E.G. Bakalbassis, A. Chatzopoulou, V.S. Melissas, M. Tsimidou, M. Tsolaki and A. Vafiadhis,  
"Ab Initio and Density Functional Theory Studies for the Explanation of the Antioxidant Activity of Certain Phenolic Acids",  
Lipids, 36, 181 - 190 (2001).
2. D. Papayannis, A.M. Kosmas, V.S. Melissas,  
"A Quantum Mechanical Study of the Structure, Vibrational Spectra, and Relative Energetics of XOOI, XOIO, and XIOO Isomers, X = Cl, Br, and I",  
Chem. Phys. Lett., 349, 299 - 306 (2001).
3. D. Papayannis, A.M. Kosmas and V.S. Melissas,  
"Quantum Mechanical Studies on the BrO + ClO Reaction",  
J. Phys. Chem. A, 105, 2209 - 2215 (2001).
4. I.G. Economou,  
"Monte Carlo Simulation of Phase Equilibria of Aqueous Systems",  
Fluid Phase Equil., 183-184, 259-269 (2001).
5. Boulougouris, G.C.; Voutsas, E.C.; Economou, I.G.; Theodorou, D.N.; Tassios, D.P.,  
"Henry's Constant Analysis for Water and Nonpolar Solvents from Experimental Data, Macroscopic Models, and Molecular Simulation",  
J. Phys. Chem. B, 105, 7792-7798 (2001).
6. Boulougouris, G.C.; Economou, I.G.; Theodorou, D.N.,

"Calculation of the chemical potential of chain molecules using the staged particle deletion scheme",

J. Chem. Phys., 115, 8231-8237 (2001).

7. Makrodimitris, K.; Papadopoulos, G.K.; Theodorou, D.N.,  
"Prediction of Permeation Properties of CO<sub>2</sub> and N<sub>2</sub> through Silicalite via Molecular Simulations",

J. Phys. Chem. B, 105, 777-788 (2001).

8. Zervopoulou, E.; Mavrantzas, V.G.; Theodorou, D.N.,  
"A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene",

J. Chem. Phys., 115, 2860-2875 (2001)

## **2000**

1. E. Voutsas, G.C. Boulougouris, I.G. Economou and D.P. Tassios,  
"Phase Equilibria of Water/Hydrocarbon Systems from two Equations of State Using the Thermodynamic Perturbation Theory",

Ind. Eng. Chem. Res., 39(3), 797-804 (2000).

2. H. Mahgerefteh, P. Saha and I.G. Economou,  
"Modeling Fluid Phase Transition Effects on Dynamic Behavior of ESDV",

AIChE J., 46(5), 997-1006 (2000).

3. I.G. Economou,  
"Lattice-Fluid Theory Prediction of High-Density Polyethylene - Branched Polyolefin Blend Miscibility",  
Macromolecules, 33(13), 4954-4960 (2000).
  
4. G.C. Boulougouris, J.R. Errington, I.G. Economou, A.Z. Panagiotopoulos and D.N. Theodorou,  
"Molecular Simulation of Phase Equilibria for Water - n-Butane and Water - n-Hexane Mixtures",  
J. Phys. Chem. B, 104(20), 4958-4963 (2000).
  
5. N.M. Zouridakis, I.G. Economou, K.P. Tzevelekos, E.S. Kikkinides,  
"Investigation of the Physicochemical Characteristics of Ancient Mortars by Static and Dynamic Studies",  
Cem. Concr. Res., 30, 1151-1155 (2000).
  
6. V.S. Melissas, E. Drougas, E.G. Bakalbassis and A.M. Kosmas, "Dynamics of the  $\text{OH} + \text{Cl}_2 \rightarrow \text{HOCl} + \text{Cl}$  Reaction: Ab Initio Investigation and Quasiclassical Trajectory Calculations of Reaction Selectivity", J. Phys. Chem. A, 104(3), 626 - 634 (2000).

## **1999**

1. G.C. Boulougouris, I.G. Economou and D.N. Theodorou,  
"On the Calculation of the Chemical Potential Using the Particle Deletion Scheme",  
Molec. Phys., 96(6), 905-913 (1999).
  
2. D. Spyriouni, I.G. Economou and D.N. Theodorou,

"Molecular Simulation of  $\alpha$ -Olefins Using a New Potential Model: Vapor-Liquid Equilibria of Pure Compounds and Mixtures",  
J. Amer. Chem. Soc., 121(14), 3407-3413 (1999).

3. T. Varzakas, I. Escudero and I.G. Economou,  
"Estimation of Endoglucanase and Lysozyme Effective Diffusion Coefficients in Polysulphone Membranes",  
J. of Biotechnology, 72(1-2), 77-83 (1999).

4. H. Mahgerefteh, P. Saha and I.G. Economou,  
"Fast Numerical Simulation for Full Bore Rupture of Pressurized Pipelines",  
AIChE J., 45(6), 1191-1201 (1999).

5. Antoniadis S.J., Samara C.T. and Theodorou D.N.  
"Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts",  
Macromolecules, 32, 8635-8644 (1999).

## **1998**

1. Antoniadis S.J., Samara C.T. and Theodorou D.N.  
"Molecular Dynamics of Atactic Polypropylene Melts",  
Macromolecules, 31, 7944-7952 (1998).

2. H. Mahgerefteh, P. Saha and I.G. Economou,  
"ESDV Performance Following Full Bore Rupture of Long Pipelines",  
The Chemical Engineer, 666, 26-28 (1998).

3. D. Spyriouni, I.G. Economou and D.N. Theodorou,  
"Molecular Simulation of the Pure n-Hexadecane Vapor-Liquid Equilibria at Elevated Temperature",  
Macromolecules, 31(4), 1430-1431 (1998).

4. D. Spyriouni, I.G. Economou and D.N. Theodorou,  
"Phase Equilibria of Mixtures Containing Chain Molecules Predicted Through a Novel Simulation Scheme",  
Phys. Rev. Lett., 80(20), 4466-4469 (1998).
  
5. G.C. Boulougouris, I.G. Economou and D.N. Theodorou,  
"Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature and Pressure Range",  
J. Phys. Chem. B, 102(6), 1029-1035 (1998).
  
6. J.R. Errington, G.C. Boulougouris, I.G. Economou, A.Z. Panagiotopoulos and D.N. Theodorou,  
"Molecular Simulation of Phase Equilibria for Water - Methane and Water - Ethane Mixtures",  
J. Phys. Chem. B, 102(44), 8865-8873 (1998).
  
7. Nikolaos P. Kopsias and D. N. Theodorou,  
"Elementary structural transitions in the amorphous Lennard-Jones solid using multidimensional transition-state theory"  
J. Chem. Phys. , 109(19) 8573 (1998).

## **1997**

1. I.G. Economou, J.L. Heidman, C. Tsonopoulos and G.M. Wilson,  
"High-Temperature Mutual Solubilities of Hydrocarbons and Water. Part III: 1-Hexene, 1-Octene, C10 - C12 Hydrocarbons",  
AIChE J., 43(2), 535-546 (1997).
  
2. I.G. Economou and C. Tsonopoulos,  
"Associating Models and Mixing Rules in Equations of State for Water-Hydrocarbon Mixtures",  
Chem. Eng. Sci., 52(4), 511-525 (1997).
  
3. H. Mahgerefteh, P. Saha and I.G. Economou,  
"A Study of the Dynamic Response of Emergency Shutdown Valves Following Full Bore Rupture of Long Pipelines",

Trans. Inst. Chem. Eng. Proc. Safety Envir. Prot., 75 (B4),201-209 (1997)

4. D. Spyriouni, I.G. Economou and D.N. Theodorou,  
"Thermodynamic of Chain Fluids from Atomistic Simulation: A Test of the Chain  
Increment Method for Chemical Potential",  
Macromolecules, 30, 4744-4755 (1997)

## **1996**

1. E.J. Maginn, A.T. Bell, and D.N. Theodorou,  
"Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulation  
Approach", J. Phys. Chem., 100, 7155-7173 (1996).

2. C.S. Chassapis, J.K. Petrou, J.H. Petropoulos and D.N. Theodorou,  
"Analysis of Computed Trajectories of Penetrant Molecules in a Simulated  
Polymeric Material",  
Macromolecules, 29, 3615-3624 (1996).

3. I.G. Economou and M.D. Donohue,  
"Equations of State for Hydrogen Bonding Systems",  
Fluid Phase Equil., 116, 518-529 (1996).

4. K. Kiyohara, D. Spyriouni, K.E. Gubbins and A.Z. Panagiotopoulos,  
"Thermodynamic Scaling Gibbs Ensemble Monte Carlo - A New Method for  
Determination of Phase Coexistence Properties of Fluids",  
Mol. Phys., 89(4), 965-974 (1996).



