ATHANASSIOS Z. PANAGIOTOPOULOS

EDUCATION

Dipl. Eng. (5-year degree) in Chemical Engineering,
National Technical University of Athens, Greece (1982)

Ph.D.,
Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA (1986)

Postdoctoral,
Physical Chemistry Laboratory, University of Oxford, United Kingdom (1986-1987)

PROFESSIONAL POSITIONS

School of Chemical Engineering, Cornell University, Ithaca, NY
Assistant Professor (1987-92), Assoc. Professor (1992-97), Professor (1998-99, on leave)

Democritus National Research Center, Athens, Greece, Visiting Scientist (1993-94, 2020)

Institute for Physical Science and Technology and Department of Chemical Engineering, University of Maryland, College Park, MD, Professor (1997-2000)

Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ
Professor (2000-2006), Director of Graduate Studies (2003-05, 2013-14), Susan Dod Brown Professor (2007-present), Department Chair (2016-2022)

SELECTED HONORS

BASF Lectureship, Wayne State U., 2021
SEAS Distinguished Teacher Award, Princeton U., 2020
Robert L. Pigford Memorial Lecturer, U. of Delaware, 2018
Keith E. Gubbins Inaugural Lecturer, N. Carolina State U., 2016
Chemical Engineering Distinguished Lecturer, Texas A&M at Qatar, 2013
American Academy of Arts and Sciences, 2012
National Academy of Engineering, 2004
J.M. Prausnitz Award for Achievement in Applied Chemical Thermodynamics, 1998
Colburn Award of the American Institute of Chemical Engineers, 1995

PROFESSIONAL AFFILIATIONS

American Institute of Chemical Engineers (elected Fellow in 2014)
American Chemical Society
American Physical Society
American Association for the Advancement of Science (elected Fellow in 2012)

EDITORIAL, ADVISORY BOARD, AND COUNCIL MEMBERSHIPS

J. Chem. Phys., Editorial Advisory Board, 2020 – 2022
Molecular Physics, Advisory Board, 2008 – 2023; Editorial Board, 2023 – present
AIChE J., Contributing Editors Board, 2012 – 2020
Midwest Integrated Center for Computational Materials Sci. Advisory Board, 2017 – present

BOOK

Essential Thermodynamics, Drios Press, 2011 (undergraduate textbook)

REFEREED PUBLICATIONS

Citation data as of Feb. 2, 2024: Google Scholar: 26,313 total citations, h=81; Web of Science: 21,449 total citations, h=72.

1. A. Z. Panagiotopoulos and S. K. Kumar, "A generalized technique to obtain pure component parameters for two-parameter equations of state," *Fluid Phase Equilibria*, **22**: 77-88 (1985). DOI: 10.1016/0378-3812(85)87012-6 *[Web of Science citations: 22]*
2. A. Z. Panagiotopoulos and R. C. Reid, "New mixing rule for cubic equations of state for highly polar, asymmetric systems," *ACS Symposium Ser.*, **300**: 571-582 (1986). DOI: 10.1021/bk-1986-0300.ch028 *[211]*
3. A. Z. Panagiotopoulos and R. C. Reid, "Multiphase high-pressure equilibria in ternary aqueous systems," *Fluid Phase Equilibria*, **29**: 525-534 (1986). DOI: 10.1016/0378-3812(86)85051-8 *[79]*
4. A. Z. Panagiotopoulos and R. C. Reid, "On the relationship between pair-wise fluctuations and thermodynamic derivatives," *J. Chem. Phys.*, **85**: 4650-4653 (1986). DOI: 10.1063/1.451761 *[19]*
5. A. Z. Panagiotopoulos, U. W. Suter, and R. C. Reid, "Phase diagrams of non-ideal fluid mixtures from Monte-Carlo simulation," *Ind. Eng. Chem. Fundam.*, **25**: 525-535 (1986). DOI: 10.1021/i100024a012 *[70]*
6. A. Z. Panagiotopoulos, R. C. Wilson, and R. C. Reid, "Phase equilibria in ternary systems with carbon dioxide, water and carboxylic acids at elevated pressures," *J. Chem. Eng. Data*, **33**: 321-327 (1988). DOI: 10.1021/je00053a028 *[27]*
7. A. Z. Panagiotopoulos and R. C. Reid, "High pressure phase equilibria in ternary mixtures with a supercritical component," *ACS Symposium Ser.*, **329**: 115-129 (1987). DOI: 10.1021/bk-1987-0329.ch010 *[31]*
8. A. Z. Panagiotopoulos, "Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble," *Mol. Phys.*, **61**: 813-826 (1987). Reprinted in the special issue "Defining Papers in Molecular Physics, 1958-2001" **100**: 237-46 (2002). DOI: 10.1080/00268978700101491 *[1,894+19]*
9. A. Z. Panagiotopoulos, "Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble," *Mol. Phys.*, **62**: 701-719 (1987). DOI: 10.1080/00268978700102501 *[285]*
10. G. B. Woods, A. Z. Panagiotopoulos, and J. S. Rowlinson, "Adsorption of fluids in model zeolite cavities," *Mol. Phys.*, **63**: 49-63 (1988). DOI: 10.1080/00268978800100051 *[124]*
11. A. Z. Panagiotopoulos, N. Quirke, M. Stapleton, and D. J. Tildesley, "Phase equilibria by simulation in the Gibbs ensemble: alternative derivation, generalization and application to mixture and membrane equilibria," *Mol. Phys.*, **63**: 527-545 (1988). DOI: 10.1080/00268978800100361 *[1,110]*
12. M. R. Stapleton, D. J. Tildesley, N. Quirke, and A. Z. Panagiotopoulos, "Phase equilibria of quadrupolar fluids by simulation in the Gibbs ensemble," *Mol. Simulation*, **2**: 147-162 (1989). DOI: 10.1080/08927028908031364 *[54]*

13. A. Z. Panagiotopoulos, "Exact calculations of fluid-phase equilibria by Monte Carlo simulation in a new statistical ensemble," *Int. J. Thermophys.* **10**: 447-457 (1989). DOI: 10.1007/BF01133541 *[107]*

14. A. Z. Panagiotopoulos, "Gibbs-ensemble Monte Carlo simulations of phase equilibria in supercritical fluid systems," *ACS Symposium Ser.*, **406**: 39-51 (1989). DOI: 10.1021/bk-1989-0406.ch004 *[12]*

15. A. Z. Panagiotopoulos and M. R. Stapleton, "The Gibbs method for calculating phase equilibria by simulation," *Fluid Phase Equilibria*, **53**: 133-141 (1989). DOI: 10.1016/0378-3812 (89)80080-9 *[38]*

16. K. E. Gubbins and A. Z. Panagiotopoulos, "Molecular Simulation," *Chem. Eng. Progress*, **85** (10): 23-27 (1989).

17. M. R. Stapleton and A. Z. Panagiotopoulos, "Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble," *J. Chem. Phys.*, **92**: 1285-93 (1990). DOI: 10.1063/1.458138 *[65]*

18. R. C. Willson, A. Z. Panagiotopoulos, and R. C. Reid, "High-pressure phase equilibria in ternary systems of propionic acid and water with ethane, SF_6, or refrigerant 13 ($CClF_3$), 23 (CF_3H) or 116 (C_2F_6)," *J. Chem. Eng. Data*, **36**: 290-293 (1991). *[2]*

19. V. I. Harismiadis, K. K. Koutras, D. P. Tassios, and A. Z. Panagiotopoulos, "How good is conformal solutions theory for phase equilibrium predictions?" *Fluid Phase Equil.*, **65**: 1-18 (1991). DOI: 10.1016/0378-3812(91)87014-Z *[87]*

20. M. E. van Leeuwen, C. J. Peters, J. de Swaan Arons, and A. Z. Panagiotopoulos, "Evaluation of a statistical-mechanical virial equation of state using Gibbs-ensemble molecular simulation," *Fluid Phase Equilibria*, **66**: 41-55 (1991). DOI: 10.1016/..5046-W *[8]*

21. M. E. van Leeuwen, C. J. Peters, J. de Swaan Arons, and A. Z. Panagiotopoulos, "Investigation of the transition to liquid-liquid immiscibility for Lennard-Jones (12,6) systems using Gibbs-ensemble molecular simulations," *Fluid Phase Equilibria*, **66**: 57-75 (1991). DOI: 10.1016/0378-3812(91)85047-X *[32]*

22. S. K. Kumar, I. Szleifer, and A. Z. Panagiotopoulos, "Determination of chemical potentials in polymeric systems from Monte Carlo simulations," *Phys. Rev. Lett.*, **66**: 2935-2938 (1991). DOI: 10.1103/PhysRevLett.66.2935 *[151]*

23. A. Z. Panagiotopoulos, "Molecular simulation of fluid-phase equilibria: simple, ionic and polymeric fluids," *Fluid Phase Equil.*, **76**: 97-112 (1992); erratum in **92**, 313 (1994). DOI: 10.1016/0378-3812(92)85080-R *[133]*

24. A. Z. Panagiotopoulos, "Direct determination of fluid phase equilibria by simulation in the Gibbs ensemble: a review," *Mol. Simulation*, **9**: 1-23 (1992). DOI: 10.1080/08...48258 *[339]*

25. I. Szleifer, E. M. O' Toole, and A. Z. Panagiotopoulos, "Monte Carlo simulation of the collapse-coil transition in homopolymers," *J. Chem. Phys.*, **97**: 6802-8 (1992). DOI: 10.1063/1.463633 *[54]*

26. I. Szleifer and A. Z. Panagiotopoulos, "Chain length and density dependence of the chemical potential of lattice polymers," *J. Chem. Phys.*, **97**: 6666-73 (1992). DOI: 10.1063/1.463671 *[22]*

27. E. M. O' Toole and A. Z. Panagiotopoulos, "Monte Carlo simulation of folding transitions of simple model proteins using a chain growth algorithm," *J. Chem. Phys.*, **97**: 8644-52 (1992). DOI: 10.1063/1.463383 *[67]*

28. A. D. Mackie, E. M. O' Toole, D. A. Hammer, and A. Z. Panagiotopoulos, "Molecular simulation of self-assembly in surfactant and protein solutions," *Fluid Phase Equil.*, **82**: 251-260 (1993). DOI: 10.1016/0378-3812(93)87149-U *[11]*

29. G. Orkoulas and A. Z. Panagiotopoulos, "Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertions," *Fluid Phase Equil.*, **83**: 223-231 (1993). DOI: 10.1016/0378-3812(93)87025-V *[10]*

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32. J. K. Johnson, A. Z. Panagiotopoulos, and K. E. Gubbins, "Reactive canonical Monte Carlo: A new simulation technique for reacting or associating fluids," *Molec. Phys.*, **81**: 717-733 (1994). DOI: 10.1080/00268979400100481 *[188]*

33. A. Z. Panagiotopoulos, "Molecular simulation of phase equilibria," NATO ASI Series E, **273**, 411-437 (1994). DOI: 10.1007/978-94-015-8295-7_16 *[17]*

34. V. I. Harismiadis, A. Z. Panagiotopoulos, and D. P. Tassios, "Phase equilibria of binary Lennard-Jones mixtures with cubic equations of state," *Fluid Phase Equilibria*, **94:** 1-18 (1994). DOI: 10.1016/0378-3812(94)87049-7 *[23]*

35. Y.-J. Sheng, A. Z. Panagiotopoulos, S. K. Kumar, and I. Szleifer, "Monte Carlo calculation of phase equilibria for a bead-spring polymeric model," *Macromolecules*, **27**: 400-406 (1994). DOI: 10.1021/ma00080a012 *[113]*

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39. A. D. Mackie, A. Z. Panagiotopoulos, D. Frenkel, and S. K. Kumar, "Constant-pressure Monte Carlo simulations for lattice models," *Europhys. Lett.*, **27**, 549-554 (1994). DOI: 10.1209/0295-5075/27/7/010 *[20]*

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41. E. M. O' Toole, R. Venkataramani, and A. Z. Panagiotopoulos, "A simple lattice model of proteins incorporating directional bonding and a structured solvent," *AIChE J.*, **41**, 954-958 (1995). DOI: 10.1002/aic.690410425 *[5]*

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44. P. C. Tsang, O. N. White, B. Y. Perigard, L. F. Vega, and A.Z. Panagiotopoulos, "Phase equilibria in ternary Lennard-Jones systems," *Fluid Phase Equil.*, **107**, 31-43 (1995); erratum in **129**, 311 (1997). DOI: 10.1016/0378-3812(94)02628-E *[31]*

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46. A.D. Mackie, A.Z. Panagiotopoulos, and S.K. Kumar, "Monte Carlo Simulations of Phase Equilibria for a Lattice Homopolymer Model," *J. Chem. Phys.*, **102**, 1014-23 (1995). DOI: 10.1063/1.469450 *[63]*

47. A.Z. Panagiotopoulos, "Gibbs ensemble techniques," NATO ASI Series C, **460**, 463-501 (1995). DOI: 10.1007/978-94-011-0065-6_11 *[59+10]*

48. Y.-J. Sheng, A.Z. Panagiotopoulos, and S.K. Kumar, "Mixing Properties of Model Polymer/Solvent Systems," *J. Chem. Phys.*, **103**, 10315-24 (1995). DOI: 10.1063/1...9869 *[7]*

49. A.Z. Panagiotopoulos, "Current Advances in Monte Carlo Methods," *Fluid Phase Equil.*, **116**, 257-266 (1996). DOI: 10.1016/0378-3812(95)02894-3 *[35]*

50. Y.-J. Sheng, A.Z. Panagiotopoulos, and S.K. Kumar, "Effect of Chain Stiffness on Polymer Phase Behavior," *Macromolecules*, **29**, 4444-6 (1996). DOI: 10.1021/ma951343y *[36]*

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54. V. I. Harismiadis, J. Vorholz, and A. Z. Panagiotopoulos, "Efficient Pressure Estimation in Molecular Simulations Without Evaluating the Virial," *J. Chem. Phys.*, **105**, 8469-70 (1996). DOI: 10.1063/1.472721 *[83]*

55. C. J. Roberts, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Liquid-liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Pure Fluid," *Phys. Rev. Lett.*, **77**, 4386-9 (1996). DOI: 10.1103/PhysRevLett.77.4386 *[117]*

56. K. Kiyohara, K. E. Gubbins, and A. Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Stockmayer Fluids," *J. Chem. Phys.*, **106**, 3338-47 (1997). 10.1063/1.473082 *[50]*

57. A. D. Mackie, A. Z. Panagiotopoulos, and I. Szleifer, "Aggregation Behavior of a Lattice Model for Amphiphiles," *Langmuir*, **13**, 5022-31 (1997). DOI: 10.1021/la961090h *[143]*

58. A.Z. Panagiotopoulos, V. Wong, and M.A. Floriano, "Phase Equilibria of Lattice Polymers from Histogram Reweighting Monte Carlo Simulations," *Macromolecules*, **31**, 912-918 (1998). DOI: 10.1021/ma971108a *[146]*

59. K. Kiyohara, K.E. Gubbins, and A.Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Water Models," *Molec. Phys.*, **94**, 803-8 (1998). DOI: 10.1080/0...67638 *[110]*

60. J.R. Errington, K. Kiyohara, K.E. Gubbins and A.Z. Panagiotopoulos, "Monte Carlo simulation of high-pressure phase equilibria in aqueous systems," *Fluid Phase Equil.*, **151**, 33-40 (1998). DOI: 10.1016/S0378-3812(98)00273-8 *[22]*

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62. 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**, 8865-73 (1998). DOI: 10.1021/jp981627v *[123]*

63. J.R. Errington and A.Z. Panagiotopoulos, "A Fixed Point Charge Model for Water Optimized to the Vapor-Liquid Coexistence Properties," *J. Phys. Chem. B*, **102**, 7470-7475 (1998). DOI: 10.1021/jp982068v *[187]*

64. J.Y. Lee, A.R.C. Baljon, R.F. Loring, and A.Z. Panagiotopoulos, "Simulation of Polymer Melt Intercalation in Layered Nanocomposites," *J. Chem. Phys.*, **109**, 10321-30 (1998). DOI: 10.1063/1.477687 *[65]*

65. G. Orkoulas and A.Z. Panagiotopoulos, "Phase Behavior of the Restricted Primitive Model and Square-Well Fluids from Monte Carlo Simulations in the Grand Canonical Ensemble," *J. Chem. Phys.*, **110**, 1581-90 (1999). DOI: 10.1063/1.477798 *[241]*

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67. M.A. Floriano, E. Caponetti, and A.Z. Panagiotopoulos, "Micellization in Model Surfactant Systems," *Langmuir*, **15**, 3143-3151 (1999). DOI: 10.1021/la9810206 *[202]*

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72. A. Z. Panagiotopoulos, "Monte Carlo Methods for Phase Equilibria," *J. Phys. Condensed Matter*, **12**, R25-R52 (2000). DOI: 10.1088/0953-8984/12/3/201 *[294+29]*

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77. A. Z. Panagiotopoulos, "On the equivalence of continuum and lattice models for fluids," *J. Chem. Phys.*, **112**, 7132-7 (2000). DOI: 10.1063/1.481307 *[76]*

78. 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**, 4958-63 (2000). DOI: 10.1021/jp994063j *[49]*

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