

NAME: Barbara N. Hale

Fall 2015

TITLE: Professor of Physics,
Senior Investigator, Cloud and Aerosol Science Laboratory
Missouri University of Science and Technology

EDUCATION: B.S., Physics, Syracuse University, 1960
Ph.D., Physics, Purdue University, 1967

ACADEMIC EXPERIENCE:

Assistant Professor of Physics, Rochester Institute of Technology, Rochester, NY, 1968-69
Visiting Assistant Professor of Mathematics, University of Missouri -Rolla, 1969-1971
Research Associate, Graduate Center for Cloud Physics Research, University of Missouri - Rolla, 1971-73
Assistant Professor of Physics and Senior Research Investigator, Graduate Center for Cloud Physics Research, University of Missouri-Rolla, 1973-77
Associate Professor and Senior Research Investigator, Graduate Center for Cloud Physics Research, University of Missouri-Rolla, 1977-1982
Professor of Physics and Senior Investigator, Cloud and Aerosol Science Laboratory, 1982-present

PROFESSIONAL AFFILIATIONS:

The American Physical Society, The American Association of Physics Teachers, The American Meteorological Society, Phi Beta Kappa, Sigma Xi, Sigma Pi Sigma, Phi Kappa Phi

AWARDS:

University of Missouri-Rolla Faculty Excellence Awards, 1986, 1987, 1989, 1990;
University of Missouri-Rolla Outstanding Teacher Award, 1989.
Chi Omega National Advisor Award, June 2000
UMR Alumni Association Faculty Advisor Award, 2002
MS&T Woman of the Year 2013
National Chi Omega Fraternity Lifetime Service Award 2014
Teaching Recommendation Spring 2015

PUBLICATIONS:

B. Hale, G. Wilemski and A. Viets, "Monte Carlo Simulations of Growth/Decay Rate Constant Ratios for Small Methanol Clusters: Application to Nucleation Data Analysis", *"Nucleation and Atmospheric Aerosols 2009"*, Edited by P. DeMott and C. O'Dowd, American Institute of Physics Conference Proceedings, 1527 NY (2013)

Barbara N. Hale and Mark Thomason, "Scaled Vapor-to-Liquid Nucleation in a Lennard-Jones System", *Phys. Rev. Lett.* **105**, 046101 (2010).

Barbara N. Hale and Gerald Wilemski, "A Comparison of Small Cluster Effects in Argon Lennard-Jones Nucleation", *"Nucleation and Atmospheric Aerosols 2009"*, Conference Proceedings, edited by J. Smolik and C. O'Dowd, University of Prague (2009)

Barbara N. Hale and Jerry Kiefer, "A Study of Scaled Nucleation in a Model Lennard-Jones System", *"Nucleation and Atmospheric Aerosols 2007"*, Conference Proceedings, edited by Colin D. O'Dowd and Paul Wagner, Springer, (2007) pp.149-152

Barbara N. Hale, "Temperature dependence of homogeneous nucleation rates for water: Near equivalence of the empirical fit of Wolk and Strey, and the scaled nucleation model", *J. Chem. Phys.* **122**, 204509 (2005).

B. N. Hale and D. J. DiMattio, "Scaling of the Nucleation Rate and a Monte Carlo Discrete Sum Approach to Water Cluster Free Energies of Formation", *J. Phys. Chem. B*, **108**, 19780 (2004).

Barbara N. Hale, "Computer Simulations, Nucleation Rate Predictions and Scaling" in *Nucleation and Atmospheric Aerosols 2004*, Edited by M. Kasahara and M. Kulmala, Kyoto University Press, Kyoto Japan, pp. 3-14 (2004)

B. N. Hale and S. M. Kathmann, "Monte Carlo Simulations of Small Sulfuric Acid – Water Clusters", *J. Phys. Chem.*, B105, 11719 (2001).

J. Kiefer and B. N. Hale, "Effective Surface Tension for Small Binary Clusters by Monte Carlo Simulation", *"Nucleation and Atmospheric Aerosols 2000"*, edited by B. N. Hale and M. Kulmala, AIP Press, Melville NY (2000) p.260.

Barbara Hale and David J. DiMaggio, "A Monte Carlo Discrete Sum (MCDS) Nucleation Rate Model for Water". *"Nucleation and Atmospheric Aerosols 2000"*, edited by B. N. Hale and M. Kulmala, AIP Press, Melville NY (2000) p. 31.

Barbara N. Hale and Gerald Wilemski, "A Scaled Nucleation Model for Ideal Binary Systems", *Chemical Physics Letters*, 305, 263 (1999)

Barbara N. Hale, "Monte Carlo Calculations of Effective Surface Tension for Small Clusters", *Aust. J. Phys.* **49**, 425 (1996)

B. N. Hale and D. J. DiMaggio, "Monte Carlo Studies of Water/Ice Adsorbed on Model AgI: Effects of Lattice Mismatch", *Nucleation and Atmospheric Aerosols*, Ed. by M. Kulmala and P. Wagner, Pergamon (Elsevier), New York, (1996), page 349.

B. N. Hale and S. M. Kathmann, "Monte Carlo Simulations of Small H₂SO₄-H₂O Clusters", *Nucleation and Atmospheric Aerosols*, Ed. by M. Kulmala and P. Wagner, Pergamon (Elsevier), New York, (1996), page 30.

James H. Taylor and Barbara N. Hale, "Monte Carlo simulations of water/ice layers on a model silver iodide substrate: comparison with bulk ice systems", *Phys. Rev. B* **47**, 9732 (1993).

Barbara N. Hale and Kyu-Kwang Han, "Microscopic liquid cluster properties and a scaled energy of formation from the vapor", in *Nucleation and Atmospheric Aerosols*, Ed. by N. Fukuta and P. E. Wagner, A. Deepak, Hampton, VA (1992), p 133.

Barbara N. Hale and Brendan Kelly, "Comments on vapor phase homogeneous nucleation of CH₃CN and a scaling law for onset supersaturation ratios", *Chem. Phys. Letters* **189**, 100 (1992)

K. Han and B. N. Hale, "Monte Carlo study of a simple model bulk ice Ih system: P-T melting behavior at constant volume", *Phys. Rev. B*, **45**, 29 (1992).

B. N. Hale, "The Scaling of Nucleation Rates", *Metallurgical Trans.* **23A**, 1863 (1992).

B. Hale, P. Kemper and J. Nuth, "Analysis of Experimental Nucleation Data for Silver and SiO Using Scaled Nucleation Theory", *J. Chem. Phys.* **91**, 4314 (1989).

P. Kemper and B. Hale, "Monte Carlo Simulations of Small Water Clusters: Effective Surface Tension", *Lecture Notes in Physics*, Volume 309, Ed. by P. E. Wagner and B. Vali, Springer-Verlag, New York (1988), p. 450.

B. Hale, "Scaled Models for Nucleation", *Lecture Notes in Physics*, Volume 309, Ed. by P. E. Wagner and B. Vali, Springer-Verlag, New York (1988), p. 323.

B. N. Hale, "Application of a Scaled Homogeneous Nucleation Rate Formalism to Experimental Data at $T \ll T_c$ ", *Phys. Rev. A* **33**, 4156 (1986).

P. Deutsch, B. Hale, R. Ward and D. Reago, "Theoretical Studies of the Structure of a Model Bulk Ice Ih Near 300 K Using a Central Force Potential Model", *J. Phys. Chem.* **87**, 4309 (1983).

P. Deutsch, B. Hale, R. Ward and D. Reago, "Structural Studies of Low Temperature Ice Ih Using a Central Force Potential Model", *J. Chem. Phys.* **78**, 5103 (1983).

R. Ward, B. Hale and S. Terrazas, "A Study of the Critical Cluster Size for Water Monolayer Clusters on a Model AgI Basal Substrate", J. Chem. Phys. **78**, 420 (1983).

R. Ward, J. Holdman and B. Hale, "Monte Carlo Studies of Water Monolayer Clusters on Substrates: Hexagonal AgI", J. Chem. Phys. **77**, 3198 (1982).

B. Hale and R. Ward, "A Monte Carlo Method for Approximating Critical Cluster Size in the Nucleation of Model Systems", J. Stat. Physics **28**, 487 (1982).

B. Hale, J. Kiefer, and C. Ward, "The Water Monomer on the Prism Face of Ice and Above a Four Layer Basal Face Ledge: an Effective Pair Potential Model", J. Chem. Phys. **75**, 1991 (1981).

J. Kiefer and B. Hale, "Studies of Water on AgI Surfaces: and Effective Pair Potential Model", J. Chem. Phys. **73**, 923 (1980).

B. Hale, J. Kiefer, S. Terrazas, and R. Ward, "Theoretical Studies of Water Adsorbed on Silver Iodide", J. Phys. Chem. **84**, 1473 (1980).

J. Kiefer and B. Hale, "The Water Monomer on the Basal Plane of Ice Ih: an Effective Pair, Central Force Potential Model of the Static Interaction", J. Chem. Phys. **67**, 3206 (1977).

J. Kassner, D. Hagen, S. Suck, P. Plummer, B. Hale et al, "Fundamental Studies on Vapor Phase Clusters", *Atmospheric Water Vapor*, Ed. A. Deepak, T. Wilkerson, and L. Ruhnke, Academic Press, New York, 1980, pp. 613-649.

P. Plummer, B. Hale, J. Kiefer, and E. Stein, "Models for Water and Ice Clusters on Simple Surfaces", Colloid and Interface Sci. **11**, 45 (1976).

B. Hale and J. Kiefer, "A Partition Function Model for Nucleation on Surfaces", J. Stat. Physics **12**, 437 (1975).

B. N. Hale and P. L. M. Plummer, "Molecular Model for Ice Clusters in a Supersaturated Vapor", J. Chem. Phys. **61**, 4012 (1974)

B. N. Hale and P. L. M. Plummer, "Comments on Nucleation Phenomena I: A Molecular Model", J. Atmos. Sci. **31**, 1615 (1974).

P. L. M. Plummer and B. N. Hale, "Molecular Model for Prenucleation Water Cluster", J. Chem. Phys. **56**, 4329 (1972).

B. Hale and K. Kikkawa, "The Differential Cross Section for Charged A Photoproduction Using the Regge Exchange Formalism", Phys. Rev. D **1**, 903 (1970).

B. Hale and A. Tubis, "Modified Phase Representation and Effects of Inelasticity in N/D Calculation of P-Wave Pion-Pion Scattering", Phys. Rev. **174**, 2074 (1968).

D. J. George, B. Hale and A. Tubis, "Modified Dispersion Relations and Scattering", Phys. Rev. **172**, 1740 (1968).

D. J. George, B. Hale and A. Tubis, "New Superconvergent Dispersion Relations for the Forward N Crossing-Even Amplitude", Phys. Rev. **168**, 1924 (1968).

RESEARCH SUPPORT:

"The Homogeneous Nucleation of Water from a Supersaturated Vapor", National Science Foundation Grant GA-32386, 1972-1974, \$40,500; with P. Plummer.

"The Molecular Model Applied to Heterogeneous Nucleation", National Science Foundation Grant GA-32386 Renewal, 1974-77, \$42,500; with P. Plummer.

Travel Grant to participate in the XVI General Assembly of the International Union of Geodesy and Geophysics, Grenoble, France, August, 1975, American Geophysical Union.

"A Molecular Model for the Theory of Ice Nucleation and Growth", NASA Contract No. NAS8-31150, 1975-1977, \$116,488; with P. Plummer.

"Molecular Models Applied to Heterogeneous Nucleation II: Studies of Water on Nucleating Surfaces", National Science Foundation Grant ATM77-12614, 1977-80, \$ 110,700; with P. Plummer.

Contributing Research Supervisor for Undergraduate Research Program Grant, 1980-1981; with D. M. Sparlin (PI).

"Molecular Models Applied to Heterogeneous Nucleation of Ice: Studies of Water on Silver Iodide and Other Ice Nucleating Substrates", National Science Foundation Grant ATM80-15790, 1980-1983, \$ 205,600; with R. Ward.

"Theoretical Studies of Microscopic De-Icing Mechanisms on Metallic Surfaces", University of Missouri Weldon Springs Grant, 1983-84, \$9,000; with S. Friberg.

"Molecular Models Applied to the Heterogeneous Nucleation of Ice: Studies of Water and Ice Layers on Silver Iodide and Other Ice Nucleating Substrates", National Science Foundation Grant ATM83-10854, 1984-1987, \$130,000.

"Ice Nucleation at a Substrate Ledge Defect", 7 CRAY-XMP hours at the National Center for Atmospheric Research, Boulder, Colorado, 1987.

"Ice Formation in Adsorbed Water Layers: Comparison with Bulk Ice Properties", 20 CRAY XMP hours at the National Center for Atmospheric Research, Boulder, Colorado, 1987.

"Ice Formation in Adsorbed Water Layers: Comparison with Bulk Ice Properties", 30 CRAY XMP hours at the National Center for Atmospheric Research, Boulder, Colorado, 1988-1989.

"Molecular Models Applied to the Heterogeneous Nucleation of Ice: Ice Formation on Surfaces", the National Science Foundation Grant ATM87-13827, 1988-1992, \$ 115,000.

"Binary Nucleation", University of Missouri Research Board Grant, 1993-1994, \$ 22,653; with John Schmitt (PI).

"Molecular Models Applied to the Nucleation of Ice", National Science Foundation Grant ATM93-07318, October 1993- June 1997, \$150,291.

"Travel and Publication Support for 15th International Conference on Nucleation and Atmospheric Aerosols", National Science Foundation, 1999-2000, \$18,000

INVITED TALKS:

B. Hale, "Applications of Mathematics to Science and Engineering", talk given to the Student Chapter of MAA, MS&T Student Mathematical Society, Rolla, Missouri, October 5, 2011.

B. N. Hale, "The Scaling of Nucleation Rates", Chemical & Biological Engineering Seminar, University of Missouri-Rolla, Rolla MO, October 2005.

B. N. Hale, "Computer Simulations, Nucleation Rate Predictions and Scaling", Lecture given at the Beijing University Chemistry Summer School, Beijing, China, August 2, 2004.

B. N. Hale, "Computer Simulations, Nucleation Rate Predictions and Scaling", Plenary Lecture at the 16th International Conference on Nucleation and Atmospheric Aerosols", Kyoto, Japan, July 26-30, 2004.

B. Hale, "A Monte Carlo Discrete Sum (MCDS) Nucleation Rate Model for Water", Colloquium, UCLA, Chemistry Department, Los Angeles, CA, January 11, 2001.

B. N. Hale, "Free energy differences for small binary clusters at fixed mole fraction and the scaling of nucleation rates for ideal binary systems", Frontier-Science Research Conference on Aerosol Science and Technology, La Jolla International School of Science, La Jolla, CA, August 16-18, 1999.

Monte Carlo Calculations of Effective Surface Tension for Small Clusters", Advanced Workshop in Atomic and Molecular Physics", Canberra, Australia, February 13, 1995.

"Scaled Models for Nucleation", Colloquium, University of Helsinki, Helsinki, Finland, November 29, 1994.

"Small Cluster Properties and a Scaled Model for Nucleation at $T \ll T_c$ ", Physics Seminar, Washington University, October 21, 1991.

"Scaled Models for Nucleation at $T \ll T_c$ ", Physics Colloquium, Purdue University, February 28, 1991

"Scaling of Nucleation Rates", G. Marshall Pound Memorial Symposium on Kinetics of Phase Transformations, held under the sponsorship of the AMS International Materials Science Division, TMS fall meeting, Detroit, October 9-11, 1990.

"Scaled Models for Nucleation", Invited Review Paper, 12th International Conference on Atmospheric Aerosol and Nucleation, Vienna, Austria, August 22-27, 1988.

Monte Carlo Simulations of Water/Ice Layers on a Model Silver Iodide Surface", University of Minnesota Supercomputer Institute, October 15, 1987.

"Monte Carlo Calculations of Free Energy Differences in Water Systems", University of Minnesota Chemical Engineering Department, June 19, 1987.

CONFERENCE PRESENTATIONS (since 2005)

B. Hale, G. Wilemski and A. Viets, "Monte Carlo Simulations of Growth/Decay Rate Constant Ratios for Small Methanol Clusters: Application to Nucleation Data Analysis", International Conference on Nucleation and Atmospheric Aerosols, Ft. Collins, CO, June 2013

G. Wilemski, B. Hale and F. Hrahsheh, "Scaling behavior and gradient theory of Methanol nucleation rates", Poster, 85th Colloid and Surface Science Symposium, June 19-22, 2011 at McGill University, Montreal, Quebec, Canada.

B. N. Hale, and G. Wilemski, "Monte Carlo simulations of growth/decay rate constant ratios for small model methanol clusters and their application to nucleation data analysis", Poster, 85th Colloid and Surface Science Symposium, June 19-22, 2011 at McGill University, Montreal, Quebec, Canada.

B. N. Hale, "Simulation-based scaling of vapor to liquid nucleation rates in a Lennard-Jones system", Talk, Nucleation Symposium, talk given at the 85th Colloid and Surface Science Symposium, June 19-22, 2011 at McGill University, Montreal, Quebec, Canada.

B. N. Hale and G. Wilemski, "Small methanol cluster growth/decay rate constant ratios and application to nucleation data analysis", American Physical Society meeting, Dallas, TX, March 2011.

B. N. Hale, "Estimates of vapor pressure for the LJ system below the triple point", American Physical Society meeting, Portland OR, March 2010.

Barbara Hale and Gerald Wilemski, "Comparison of Small Cluster Effects in Argon Lennard-Jones Nucleation", 18th International Conference on Nucleation and Atmospheric Aerosols, Prague, Czech Republic, 10-14 August 2009.

B. N. Hale, T. Mahler and J. Kiefer, "Scaled Nucleation in a Lennard-Jones System", American Physical Society meeting, New Orleans, LA, March 2008.

B. N. Hale and J. Kiefer, "A Study of Scaled Nucleation in a Model Lennard-Jones System", 17th International Conference on Nucleation and Atmospheric Aerosols, Galway, Ireland, 12-17 August 2007.

B. N. Hale, "Analysis of argon nucleation rates and theoretical model predictions", Colloid and Surface Science Symposium, Boulder CO, June 18-21, 2006.

B. N. Hale, "Computer Simulations, Nucleation Rate Predictions and Scaling", American Physical Society meeting, Los Angeles CA, March 2005.

B. N. Hale, "Application of a scaled model for heterogeneous nucleation of ice from the liquid", American Physical Society meeting, Minneapolis, March 2000.

SERVICE TO NATIONAL ORGANIZATIONS AND OTHER UNIVERSITIES:

Chairman, National Science Foundation Review Panel: Graduate Fellowships in Physics and Astronomy, Washington, D.C., February, 1988, 1989; panel member in 1986, and 1987.

Dean's Advisory Council for the School of Science, Purdue University, 1993-1996.

Referee for National Science Foundation Proposals, the Physical Review, Physical Review Letters, Journal of Physical Chemistry, Chemical Physics Letters, Journal of Physical Chemistry.

Opponent (External Reviewer) for Ph.D. thesis of Evgeni L. Zapadinsky, "Simulations of Nucleation Phenomena", Physics Department, University of Helsinki, Helsinki, Finland, November 26, 1994.

Chair, 15th International Conference on Nucleation and Atmospheric Aerosols (ICNAA), University of Missouri Rolla, Rolla MO USA, August 6-11, 2000

International Committee on Nucleation and Atmospheric Aerosols, 1996-2000, 2000-2004, 2009-present.

Editor, "Nucleation and Atmospheric Aerosols 2000", American Institute of Physics, August 2000

Speaker, St. Louis Chi Omega Alumnae Banquet, April 7, 2001, St. Louis, MO

Mary Love Collins Scholarship Review Committee, Chi Omega Fraternity, Memphis, TN, 2008 -2015

Elizabeth Orman Scholarship Review Committee, Chi Omega Fraternity, Memphis, TN, 2002.

International Review Panel for University of Helsinki Physics and Astronomy program, 2005.

Chair, International Committee on Nucleation and Atmospheric Aerosols, June 2013- June 2021.

Faculty Advisor, Eta Kappa Chapter of Chi Omega, Missouri S & T, 1979 – present.

Treasurer, House Corporation for Eta Kappa Chapter of Chi Omega, Missouri S & T, 1979-2008.

President, House Corporation for Eta Kappa Chapter of Chi Omega, Missouri S & T, 2010-present.

Treasurer, House Corporation, Upsilon Alpha Chapter of Chi Omega, Syracuse University, 2013 – present.