



School of Chemical Engineering



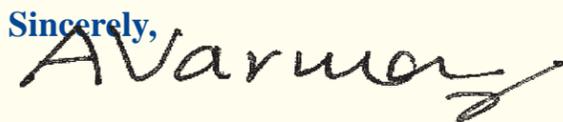
PROFESSIONAL ACTIVITY REPORT
2005 - 2006

School of Chemical Engineering Purdue University

Message from the Head

These are exciting times for Purdue and for the School of Chemical Engineering! The University has made great strides toward achieving the goals set out by the President's bold strategic plan, which includes adding 300 new faculty positions, \$600 million for construction of new academic buildings, and a \$1.5 billion capital campaign. Simultaneously, the School of Chemical Engineering has seen the completion of a major 100,000 square foot addition to its facilities in October 2004—Forney Hall, and attracted nine top-flight researchers and educators to the faculty including three members of the National Academy of Engineering. The School faculty has made significant contributions in field-defining research in key areas of national needs—from research at the nano-scale to helping develop energy sources for the future. In the following research activity report for 2005-2006, you will read about these accomplishments, including the establishment of a \$15 million NSF Engineering Research Center (ERC) on Structured Organic Composites for pharmaceutical, foods and agricultural products, along with three collaborating universities. See too the vibrancy of the program with our balance of young researchers blending with the experience of those with decades of creativity. The faculty continue to be active in professional societies, journal and book series editorships, and service on academic, industrial and governmental scientific advisory boards. They serve at all levels of professional and national responsibility, and are in great demand as lecturers in forums around the world. As challenges arise, whether in energy, nanotechnology, biotechnology, healthcare or advanced materials, the faculty of the School of Chemical Engineering at Purdue University are poised to provide the expertise and solutions.

Sincerely,



Arvind Varma
R. Games Slayter Distinguished Professor
Head, School of Chemical Engineering



Forney Hall of Chemical Engineering

School of Chemical Engineering Purdue University

PROFESSIONAL ACTIVITY REPORT 2005 - 2006

4 Research Frontiers

The Faculty

5 Rakesh Agrawal

Winthrop E. Stone Distinguished Professor

5 Chelsey D. Baertsch

6 Osman Basaran

Reilly Professor of Fluid Mechanics and Professor of Chemical Engineering

6 Stephen P. Beaudoin

7 James M. Caruthers

7 David S. Corti

8 W. Nicholas Delgass

8 Elias I. Franses

9 Robert E. Hanneman

9 Michael T. Harris

10 Hugh W. Hillhouse

10 R. Neal Houze

11 Sangtae Kim

Donald W. Feddersen Distinguished Professor

12 Gil Lee

12 Julie Liu

13 John A. Morgan

13 Joseph F. Pekny

14 R. Byron Pipes

John Leighton Bray Distinguished Professor of Engineering

14 Doraiswami Ramkrishna

H. C. Peffer Distinguished Professor and Associate Head

15 Gintaras V. Reklaitis

Edward W. Comings Professor

15 Fabio H. Ribeiro

16 Kendall T. Thomson

16 Arvind Varma

R. Games Slayter Distinguished Professor and Head

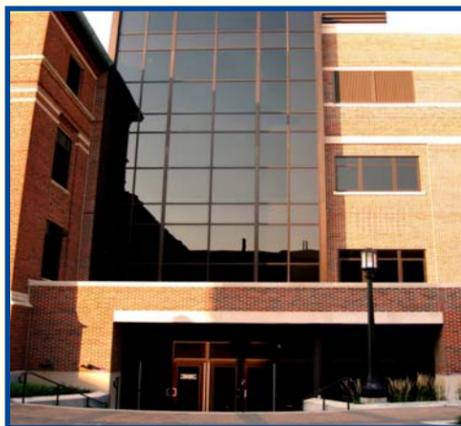
17 Venkat Venkatasubramanian

17 Nien-Hwa Linda Wang

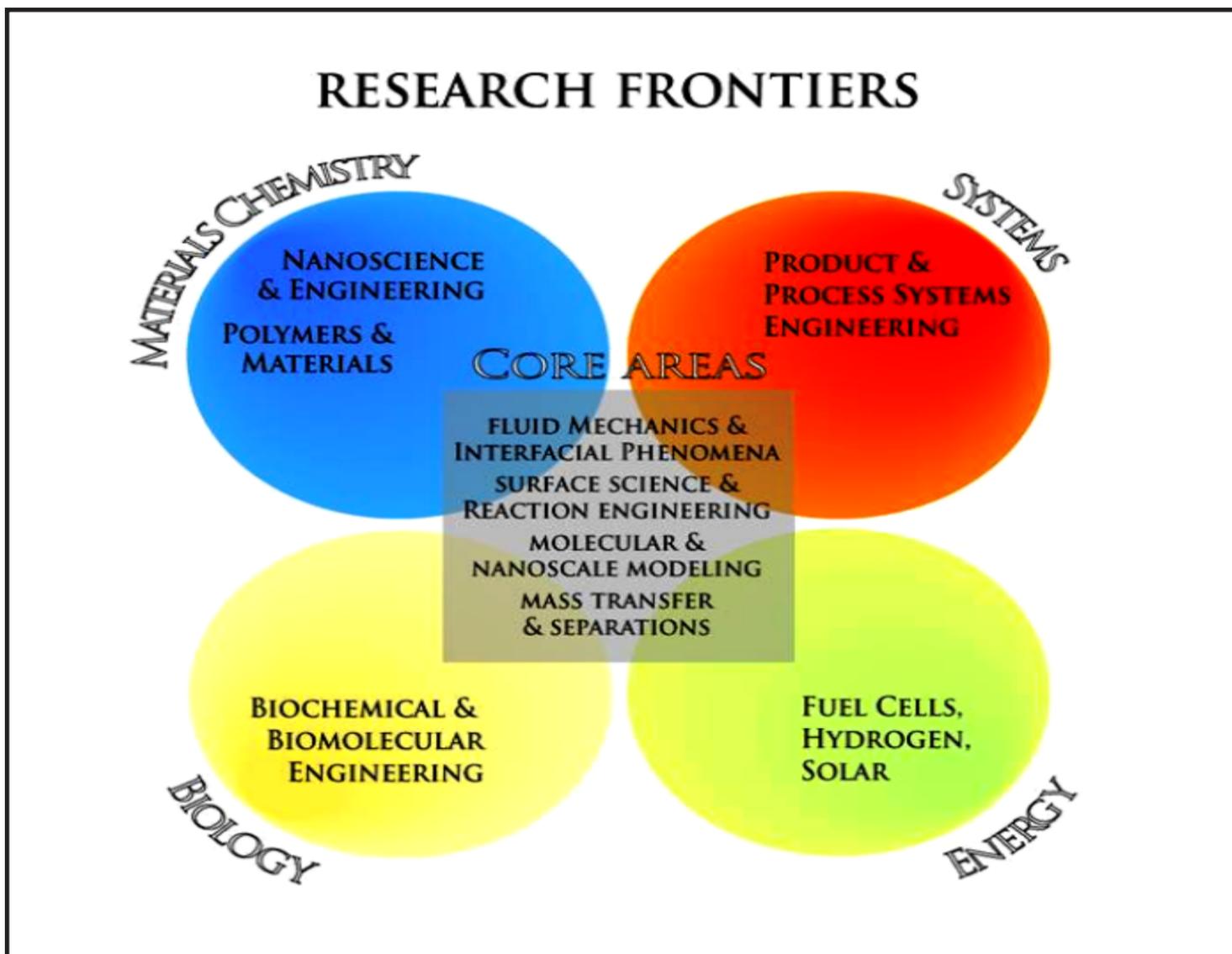
18 Phillip C. Wankat

C. L. Lovell Distinguished Professor

18 You-Yeon Won



School of Chemical Engineering



Faculty Technical Areas

Biochemical & Biomolecular Engineering

Beaudoin, Franes, Kim, Lee, Liu, Morgan, Ramkrishna, Wang

Energy

Agrawal, Baertsch, Caruthers, Delgass, Hillhouse, Morgan, Ribeiro, Varma

Fluid Mechanics & Interfacial Phenomena

Basaran, Beaudoin, Corti, Franes, Harris, Houze, Kim

Mass Transfer & Separations

Agrawal, Franes, Hillhouse, Thomson, Wang, Wankat

Molecular & Nanoscale Modeling

Corti, Harris, Thomson, Won

Nanoscience & Engineering

Beaudoin, Harris, Hillhouse, Lee, Ribeiro, Thomson, Won

Polymers & Materials

Caruthers, Hillhouse, Pipes, Varma, Won

Product & Process Systems Engineering

Agrawal, Caruthers, Kim, Pekny, Reklaitis, Venkatasubramanian

Surface Science & Reaction Engineering

Baertsch, Delgass, Ramkrishna, Ribeiro, Thomson, Varma



Rakesh Agrawal

Ph.D., Massachusetts Institute of Technology, 1980

*Winthrop E. Stone Distinguished Professor
National Academy of Engineering*

AICHE Institute Lecturer (2005)

AICHE Chemical Engineering Practice Award (2006)

Research Areas

Energy transformation and use issues for solar, coal, biomass and hydrogen economy; Novel separation processes using distillation, membranes and adsorption; Process development, cryogenics and gas liquefaction processes.

Selected Professional Activities

Consulting Editor, Separations, AIChE Journal
Advisory Council Member, School of Chemical and Biochemical Engineering, Cornell University
Member, NAE Peer Committee, Chemical Engineering Section
Member, AIChE Energy Commission
Member, NRC Board on Energy and Environmental Sciences
Member, AIChE Board of Directors

Selected Invited Lectures

“Hydrogen As An Energy Carrier – Its Promises and Challenges,” Othmer Department of Chemical Sciences and Engineering, Polytechnic University, New York, 2005.

“Synthesis of Multicomponent Distillation Column Configurations,” Department of Chemical Engineering, Clarkson University, Potsdam, NY, 2005.

“The Challenges in the Synthesis of Multicomponent Separation Configurations in Chemical Industry,” University of Colorado, Boulder, CO., 2006.

“Separation: Perspective of a Process Developer/Designer,” Department of Chemical Engineering, Tianjin University, Tianjin, China, May 2006.

“Energy Supply Challenges & Opportunities,” Peking Univ., Beijing, May 2006.

“Separation: Perspective of a Process Developer/Designer,” Department of Chemical Engineering, Tsinghua University, Beijing, China, May 2006.

Selected Publications

“Hydrogen Economy – An Opportunity for Chemical Engineers?” R. Agrawal, M. Offutt and M.P. Ramage, AIChE J, 51 (6), 1582 (2005) (An invited perspective article).

[Editor: The most downloaded article in 2006 and second most downloaded article in the AIChE Journal’s history]

“Separation Research Needs for the 21st Century”, R.D. Noble and R. Agrawal, Ind. Eng. Chem. Res., 44, 2887 (2005). (An invited commentary article).

[Editor: The most downloaded I&EC Research Journal article in 2006]

Selected Conference Presentations

“Formulation of Search Spaces for Separation Networks,” A. Giridhar, V. Venkatasubramanian, R. Agrawal, AIChE Annual National Meeting, Nov. 2005, Cincinnati, OH.

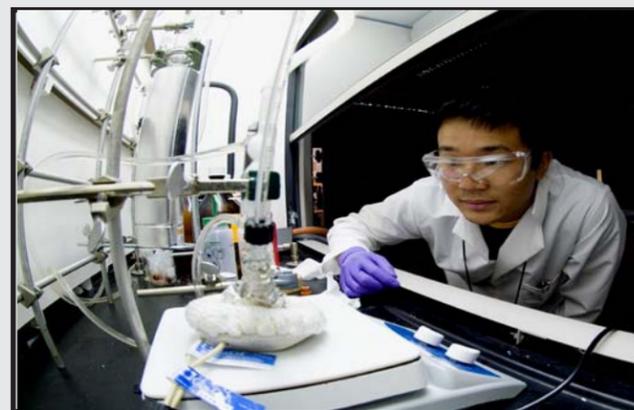
“Hydrogen As An Energy Carrier – Its Promises and Challenges,” Opening Plenary Lecture, International Chemical Engineering Conference – VI, Tec de Monterrey, Mexico, 2005

“Separation: Perspective of a Process Developer/Designer,” Invited Keynote Lecture at the ACS Symposium, San Diego, CA, 2005

“Separation: Perspective of a Process Developer/Designer,” Invited Keynote Lecture at the China/US/Japan Joint Chemical Engineering Conference, Beijing, China, October 2005.

“Energy Supply Challenges and Opportunities,” Institute Lecture, AIChE Annual Meeting, Cincinnati, 2005

“Energy Supply Challenges and Opportunities for Chemical Engineers,” Invited Plenary Lecture at the 4th Pacific Basin Conference on Adsorption Science and Technology, Tianjin, China, 2006.



Chelsey D. Baertsch

Ph.D. University of California at Berkeley, 2001

Assistant Professor

Research Areas

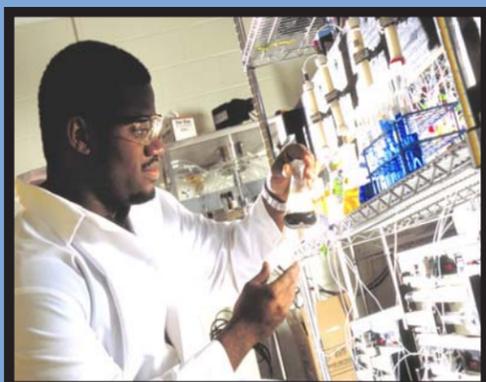
Heterogeneous Catalysis, Microchemical Systems (MEMS)

Selected Professional Activities

American Institute of Chemical Engineers (AIChE)
2006 Annual Meeting, San Francisco, CA

Chair for two Sessions:
In-situ and Operando Spectroscopy of Catalysts

Vice Chair for Session: Fundamentals of Oxide Catalysts





Osman Basaran

Ph.D, University of Minnesota, 1984

*Reilly Professor of Fluid Mechanics
and Professor of Chemical Engineering*

Director, Graduate Studies

Research Areas

Fluid Mechanics, Rheology, Drop Dynamics, Interfacial Phenomena, Finite Element Computational Analysis, Ink-jet printing, MEMS, Electroseparations

Selected Professional Activities

Member, Board of Directors, International Society for Coating Science and Technology, 1996-present.

Secretary, International Society for Coating Science and Technology, 2002-present



Selected Invited Lectures

“Small-scale flows exhibiting singularity formation, interface rupture, and unexpected dynamics,” Department of Chemical and Biomolecular Engineering, University of Maryland-College Park, College Park, Maryland, December 13, 2005.

Basaran, O. A., “Drop and Jet Breakup: What Can One Learn about Coating Stents from Ink Jet Printing and Leaky Faucets?” Guidant Corporation, Santa Clara, California, February 15, 2005.

Selected Publications

Dingle, N. M., Tjiptowidjojo, K., Basaran, O. A., and Harris, M. T. 2005 A finite element based algorithm for determining interfacial tension from pendant drop profiles. *J. Colloid Interface Sci.* 286, 647-660.

Yildirim, O. E., Xu, Q., and Basaran, O. A. 2005 Analysis of the drop weight method. *Phys. Fluids.* 17, 062107.

Liao, Y.-C., Franses, E. I., and Basaran, O. A. Deformation and breakup of a stretching liquid bridge covered with an insoluble surfactant monolayer. Accepted for publication in *Phys. Fluids*.

Suryo, R. and Basaran, O. A. Dripping without gravity. Accepted for publication in *Phys. Rev. Lett.*

Selected Conference Presentations

Liao, Y. -C., Franses, E. I., and Basaran, O. A., “Dynamics and Breakup of Stretching Bridges of Surfactant-Laden Liquids,” AIChE 2005 Annual Meeting, October 31-November 4, 2005, Cincinnati, Ohio.

Collins, R. T., Harris, M. T., and Basaran, O. A., “Interface Rupture and Formation of Finite Time Singularities in an Electric Field,” AIChE 2005 Annual Meeting, October 31-November 4, 2005, Cincinnati, Ohio.

Yeoh, H. J., Subramani, H. J., Suryo, R., Xu, Q., Ambravaneswaran, B., and Basaran, O. A., “Simplicity and Complexity of a Dripping Faucet,” 58th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), November 20-22, 2005, Chicago, Illinois.

Suryo, R. and Basaran, O. A., “Bubble Formation in a Quiescent Liquid,” 58th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), November 20-22, 2005, Chicago, Illinois.

Doshi, P., Suryo, R., Collins, R. T., Harris, M. T., and Basaran, O. A., “Unexpected Breakup Dynamics of Compound Jets,” 58th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), November 20-22, 2005, Chicago, Illinois.

Subramani, H. J., Liao, Y. -C., Franses, E. I., and Basaran, O. A., “Dynamics of Drop Formation of Surfactant-Containing Liquids,” 58th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), November 20-22, 2005, Chicago, Illinois.



Stephen P. Beaudoin

Ph.D, North Carolina State University, 1995

Professor

*Inaugural recipient, Excellence in Teaching Award
sponsored by the Purdue Student Government
and the Office of the Provost, 2005*

Research Areas

Particle and Thin Film Adhesion, Electronic Materials, Chemical Mechanical Polishing, Biosensors

Selected Professional Activities

Associate Editor, *IEEE Transactions on Semiconductor Manufacturing*
Vice President, Particle Division, Adhesion Society
Executive Committee and Governing Board, Dielectric Sciences and Technology Division, Electrochemical Society
Director, Undergraduate Recruiting, Purdue School of Chemical Engineering
Member, Purdue University Provost’s Diversity Leadership Group

Selected Invited Lectures

Beaudoin, S., “Particle Adhesion during Microelectronic Manufacturing,” Eighth International Symposium on Ultraclean Processing of Silicon Surfaces, Antwerp, Belgium, September (2006).

Kumar, G., Smith, S., Ramamoorthy, A., Eschbach, F., Salib, M., and Beaudoin, S., “Scaling of the Adhesion between Particles and Surfaces from Micron Scale to the Nanometer Scale for Photomask Cleaning Applications,” Fourth International Extreme Ultra Violet Lithography (EUVL) Symposium, sponsored by International SEMATECH, San Diego, CA, October (2005).

Kumar, G., Smith, S., and Beaudoin, S., “Particle Adhesion to Advanced Lithographic Materials,” SEMATECH Mask Cleaning Workshop, Monterey, CA, September (2005).

Kumar, G., Smith, S., and Beaudoin, S., “Multiscale Representations of Particle Adhesion,” Department of Chemical Engineering Seminar Series,

Selected Publications

Eichenlaub, S., Kumar, G., and Beaudoin, S., “A Modeling Approach to Describe the Adhesion of Rough Asymmetric Particles to Surfaces,” *Journal of Colloid and Interface Science*, 299(2), 656-664 (2006).

Kumar, G. and Beaudoin, S., “Undercut Removal of Micron-Scale Particles from Surfaces,” *J. of Electrochemical Society*, 153, G175-G181 (2006).

Pruden, K. and Beaudoin, S., “Downstream Microwave Ammonia Plasma Treatment of Parylene-C,” *J. of Vacuum Science and Technology A*, 23, 1605-1609 (2005).

Masson, J.-F., Battaglia, T. M., Davidson, M. J., Kim, Y.-C., Prakash, A. M., Beaudoin, S. P., Booksh, K. S., “Biocompatible Polymers for Antibody Support on Gold Surfaces,” *Talanta*, 67(5), 918-925 (2005).

Pruden, K. and Beaudoin, S., “Downstream Microwave Ammonia Plasma Treatment of Polydimethylsiloxane,” *J. of Vacuum Science and Technology A*, 23(1),208-214 (2005).

Selected Conference Presentations

Kumar, G., Smith, S., and Beaudoin, S., “Scaling of the Adhesion between Particles and Surfaces from Micron-Scale to the Nanometer Scale,” American Institute of Chemical Engineers Annual Meeting, November (2005).

Kumar, G., Eichenlaub, S., Kelchner, J., Graham, S., and Beaudoin, S., “Study of Particle Adhesion in Chemical Mechanical Planarization,” Adhesion Society Annual Meeting, February (2005).

Kumar, G., Smith, S., and Beaudoin, S., “Adhesion of Particles to Surfaces - Scaling from the Micron to the Nanometer Size,” Adhesion Society Annual Meeting, February (2006).



James M. Caruthers

Ph.D, Massachusetts Institute of Technology, 1977

Professor

Research Areas

Materials Design, Nonlinear Viscoelasticity of Polymers, Glass-to-Rubber Transition, Engineering Elastomers, Catalyst Design, Bioinformatics

Selected Professional Activities

Director of Center of Integrated Materials and Product Design (CIMProD)

Selected Invited Lectures

“Continuum and Meso-scope Models for the Nonlinear Relaxation Behavior of Glassy Polymers,” Symposium on Glassy Polymers, Polymer Physics Division, American Physical Society, Los Angeles, CA, March, 2005.



Selected Publications

A Bhan, S.-H. Hsu, G. Blau, J.M. Caruthers, V. Venkatasubramanian and W.N. Delgass, “Microkinetic Modeling of Propane Aromatization,” *J. Catalysis*, 235 (1): 35-51, 2005.

R. Sharma, A. Goyal, J.M. Caruthers and Y.-Y. Won, “Inhibitive Chain Transfer to Ligand in the ATRP of n-Butyl Acrylate,” *Macromolecules*, 39(14), 4680-4689, 2006

K. Phomphrai, A. E. Fenwick, S. Sharma, P. E. Fanwick, J. M. Caruthers, W. N. Delgass, M. M. Abu-Omar and I. P. Rothwell “Diverse Pathways of Activation and Deactivation of Half-Sandwich Aryloxiide Titanium Polymerization Catalysts,” *Organometallics* 25(1), 214-220, 2006.

Selected Conference Presentations

A. Goyal, P. Patkar, J. Fulk and J. M. Caruthers, “AFundamental Kinetic Model for Vulcanization of Accelerated Sulfur Vulcanization of Elastomers,” ACS Rubber Division, Paper No. 26, May, 2005.

“Local Energy Exchange Model for Predicting Super-Arrhenian Behavior,” G. Medvedev and J. M. Caruthers, 76th Annual Society of Rheology Meeting, Lubbock, TX, February, 2005.

“Computational Modeling of Olefin Polymerization by Titanium Aryloxiide Catalysts,” T.Manz, K. Thomson, J.M. Caruthers, AIChE Annual Meeting, Cincinnati, OH, Nov. 2005.

“Application of a Thermoviscoelastic Model to Enthalpy Relaxation of Polycarbonate,” P. Shrikhande, J. M. O’Reilly, G. Medvedev and James M. Caruthers, 77th Society of Rheology Meeting, Vancouver, British Columbia, Oct. 17-20, 2005.

“The Effect of Amines Catalyst on Benzothiazole Accelerated Sulfur Vulcanization,” A. Goyal, P. Patkar, J. Fulk, V. Venkatasubramanian and J. M. Caruthers, AIChE Annual Meeting, Cincinnati, OH, Nov. 2005.

“A Cyber-Infrastructure for Catalysis Science,” J.M. Caruthers, W.N. Delgass, M. McLennan, B. Krishnamurthy, S. Nandi, L. Delgass, H. Wang, L.L. Arns, S.R. Dunlop, S.-H. Hsu, M.E. Lasinski, S. Orcun, G.E. Blau, A. Goyal, J. Cao and S.P. Midkiff, AIChE Annual Meeting, San Francisco, Nov. 2006.



David S. Corti

Ph.D, Princeton University, 1997

Associate Professor

Research Interests

Molecular Thermodynamics, Metastable Liquids, Nucleation Phenomena, Colloidal Dispersions, Computer Simulation Techniques

Selected Professional Activities

Conference Organizer, 2005 Midwest Thermodynamics and Statistical Mechanics Meeting, May 26-27, Purdue University, West Lafayette, IN.

Session co-chair, “Supercooled Liquids and Nucleation,” AIChE National Meeting, Cincinnati, OH, November 2005.

Session chair, “Nucleation and Growth,” AIChE National Meeting, San Francisco, CA, November 2006.

Selected Invited Lectures

D. S. Corti, “Molecular Simulations in the Isothermal-Isobaric Ensemble: The Requirement of a ‘Shell’ Particle,” Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, November 17, 2005.

Selected Publications

D. W. Siderius and D. S. Corti, 2005, “Extension of Scaled Particle Theory to Inhomogeneous Hard Particle Fluids. I. Cavity Growth at a Hard Wall,” *Phys. Rev. E*. 71, 036141(1-12).

D. W. Siderius and D. S. Corti, 2005, “Extension of Scaled Particle Theory to Inhomogeneous Hard Particle Fluids. II. Theory and Simulation of Fluid Structure Surrounding a Cavity that Intersects a Hard Wall,” *Phys. Rev. E*. 71, 036142(1-12).

M. J. Uline and D. S. Corti, 2005, “Molecular Dynamics in the Isothermal-Isobaric Ensemble: The Requirement of a ‘Shell’ Molecule. I. Theory and Phase Space Analysis,” *J. Chem. Phys.* 123, 164101(1-14).

D. W. Siderius and D. S. Corti, 2006, “Thermodynamically Consistent Adaptation of Scaled Particle Theory to an Arbitrary Hard Sphere Equation of State,” Eduardo Glandt Festschrift, *Ind. Chem. Eng. Res.* 45, 5489-5500 (invited paper).

M. J. Uline and D. S. Corti, 2006, “The Ammonia Synthesis Reaction: An Exception to the Le Chatelier Principle and Effects of Nonideality,” *J. Chem. Educ.* 83, 138-144.

Selected Conference Presentations

D. Siderius and D. S. Corti, “Investigation of the Role of Geometry and Fluid Structure in the Description of Depletion Forces via Scaled Particle Theory based Integral Equations for Hard Sphere Fluids,” 79th ACS Colloid & Surface Science Symposium, Potsdam, NY, June 2005.

M. Uline and D. S. Corti, “The Role of Critical Cavities in Homogeneous Bubble Nucleation,” AIChE National Meeting, Cincinnati, OH, Nov 2005.

D. Siderius and D. S. Corti, “Investigation of Role of Geometry and Fluid Structure in Description of Depletion Forces Via Scaled Particle Theory-Based Integral Equations for Hard Sphere Fluids,” AIChE National Meeting, Nov 2005.

M. Uline and D. S. Corti, “Influence of Critical Cavities on Homogeneous Bubble Nucleation: A New Picture of Bubble Formation?” Midwest Thermodynamics and Statistical Mechanics Conference, Akron, OH, May '06.

D. Siderius and D. S. Corti, “Geometric Model of Depletion Forces in Hard-Sphere Colloidal Dispersions Exposed to Various Surfaces,” 80th ACS Colloid & Surface Science Symposium, Boulder, CO, June 2006.

M. Uline and D. S. Corti, “The Influence of Critical Cavities on Homogeneous Bubble Nucleation: A New Picture of Bubble Formation?” 80th ACS Colloid & Surface Science Symposium, Boulder, CO, June 2006.



W. Nicholas Delgass

Ph.D., Stanford, 1969

Professor

New York Catalysis Society Excellence in Catalysis Award, 2006

Research Areas

Heterogeneous Catalysis, Transient Kinetics, Catalyst Design and Characterization

Selected Professional Activities

Director, Catalysis and Reaction Engineering Division of AIChE, 2006-09
Editorial Board, *Journal of Catalysis* (1999 - present)
Chairman, Symposium Catalyst Design using High Throughput Experimentation, AIChE Annual Meeting, Cincinnati, OH, October 31, 2005
Co-Chairman, Symposium on High Throughput Screening for Catalysts and Processes, North American Symposium on Chemical Reaction Engineering, Houston, TX, Feb 4-7, 2007

Selected Invited Lectures

"The Chemistry and Engineering of Catalytic Reactions." Department of Chemistry, Wabash College, Crawfordsville, IN, January 25, 2005.

"Catalyst Design by Discovery Informatics," Department of Chemical Engineering, The State University at Buffalo, Buffalo, NY, February 23, 2005.

"Of Chokecherries and Catalysis," Seminar in honor of M. Albert Vannice, Department of Chemical Engineering, The Pennsylvania State University, December 8, 2005.

"Discovery Informatics-Design of Single Site Olefin Polymerization Catalysts," W. N. Delgass, J. M. Caruthers, M. M. Abu-Omar, K. T. Thomson, V. Venkatasubramanian, G. E. Blau, K. Phomphrai, G. Medvedev, S. Sharma, T. Manz, J. Haq, K. Novstrup, B. Krishnamurthy, ExxonMobil, Clinton, NJ, April 11, 2006.

"Descriptors for the Design of Olefin Polymerization Catalysts," Seminar, University of Delaware, Newark, DE, May 8, 2006.

"Model-Based Approach to Catalyst Design," 2006 Excellence in Catalysis Award Lecture, Catalysis Society of Metropolitan New York, Somerset, NJ, May 24, 2006.

Selected Publications

Mulla, S. S., N. Chen, L. Cumarantunge, G.E. Blau, D.Y. Zemlyanov, W.N. Delgass, W.S. Epling, F.H. Ribeiro, "Reaction of NO and O₂ to NO₂ on Pt: Kinetics and catalyst deactivation," *J. Catal.* 241 (2006) 389-399

Joshi, A. M., W. N. Delgass, and K.T. Thomson, "Adsorption of Small Au_n (n=1-5) and Au-Pd Clusters inside the TS-1 and S-1 pores," *J. Phys. Chem. B*, 110, 16439-16451 (2006).

B. Taylor, J.Lauterbach, G. E. Blau and W. N. Delgass, "Reaction Kinetic Analysis of the Gas-Phase Epoxidation of Propylene over Au/TS-1," *J. Catal.*, 242, 142-152 (2006)

Wells, D. H. Jr, A. M. Joshi, W. N. Delgass, K.I T. Thomson, "A Quantum Chemical Comparison of Various Propylene Epoxidation Mechanisms Using H₂O₂ and TS-1 Catalyst," *J. Phys. Chem. B*, accepted.

Selected Conference Presentations

"Modeling Propane Aromatization over ZSM-5 based Catalysts," W. N. Delgass, A. Bhan, G. Krishnamurthy, S.-H. Hsu, B. Krishnamurthy, G. Blau, J. Caruthers, and V.Venkatasubramanian, ACS Annual Meeting, San Diego, CA March 14, 2005.

"Toward Catalyst Design by Discovery Informatics," W. N. Delgass, J. M. Caruthers, V. Venkatasubramanian, K. T. Thomson, G. E. Blau, M. M.Abu-Omar, K. Phomphrai, G. Medvedev, T. Manz, S. Sharma, J. Haq, B. Krishnamurthy, K. Novstrup, A. Bhan, G. Krishnamurthy, S.-H. Hsu, Keynote talk, 19th North American Catalysis Society Meeting, May, 2005.

"The Nature of the Active Sites in Au/TS-1 Catalysts for Propene Epoxidation by Oxygen and Hydrogen," B. Taylor, L. Cumarantunge, A. M. Joshi, K.T. Thomson, and W. N. Delgass, ACS Meeting, Potsdam, NY, June 14, 2005.

"Discovery Informatics For Design Of Single Site Olefin Polymerization Catalysts," W. N. Delgass, J. M. Caruthers, M. M. Abu-Omar, K. T. Thomson, V. Venkatasubramanian, G. E. Blau, K. Phomphrai, G. Medvedev, S. Sharma, T. Manz, J. Haq, K. Novstrup, and B. Krishnamurthy, ACS National Meeting, Atlanta, GA, March 30, 2006.

"Model-Based Design of Single Site Olefin Polymerization Catalysts," W. N. Delgass, J. M. Caruthers, M. M. Abu-Omar, K. T. Thomson, V. Venkatasubramanian, G. E. Blau, K. Phomphrai, G. Medvedev, C. Stanciu, S. Sharma, T. A. Manz, J. Haq, K. A. Novstrup, and B. Krishnamurthy, AIChE Annual Meeting, San Francisco, CA, November 15, 2006.



Elias I. Franses

PhD, Minnesota, 1979

Professor

Research Areas

Adsorption and Dynamics of Surfactants and Proteins at Interfaces, Thin Organic Coatings, Infrared Spectroscopy and Ellipsometry of Thin Films

Selected Professional Activities

Co-Chair, "Transport at Interfaces I and II," AIChE Annual Meeting, San Francisco, CA, November 2006, with Prof. A. Chauhan.
Co-Chair, "Nanoscale Modeling of Interfacial Systems," with Prof. P. Tassel, AIChE Annual Meeting, Cincinnati, Ohio, October 2005,
Member, two NSF panels, 2005.

Selected Invited Lectures

Chemical Engineering, Wayne State University, Detroit, Michigan, October 2005, "Dynamics, Direct Probing, and Mechanisms of Adsorption of Lipids and Serum Proteins at Air-Water Interfaces. Implications for Alveolar Lung Diseases."

Sandia National Laboratories, Livermore, California, January 2006, "Physically Self-Assembled Monolayers (PSAMs) of Lecithin Lipids on Hydrophilic Silicon Oxide Interfaces."

Selected Publications

Kasat, R. B., Zvinevich, Y., Hillhouse, H. W., Thomson, K. T., Wang, N-H. L., and Franses, E. I., "Direct probing of Sorbent-Solvent Interactions for Amylose Tris(3,5-dimethylphenylcarbonate) Using Infrared Spectroscopy, X-ray Diffraction, Solid-State NMR, and DFT Modeling," *J. Phys. Chem. B*, 100, 14114-14122 (2006).

Yu, C.-M., Chin, C.Y. Franses, E. I., and Wang, N.-H. L., "In-Situ Probing of Insulin Aggregation in Chromatography Effluents with Spectroturbidimetry," *J. Colloid Interf. Sci.*, 299, 733-739 (2006).

Liao, Y.-C., Basaran, O.A., and Franses, E. I., "The Effects of Dynamic Surface Tension and Fluid Flow on the Oscillations of a Supported Bubble," *Colloids Surfaces A*, 282, 183-202 (2006); invited article for Special Issue in Honor of I.B. Ivanov.

Phang, T.-Z., and Franses, E. I., "Physically Self-Assembled Monolayers (PSAMs) of Lecithin Lipids on Hydrophilic Silicon Oxide Interfaces," *Langmuir*, 22, 1609-1618(2006).

Kim, S. H., and Franses, E. I., "Competitive Adsorption of Fibrinogen and Dipalmitoylphosphatidylcholine of the Air/Aqueous Interface," *J. Colloid Interf. Sci.*, 295, 84-92 (2006)

Selected Conference Presentations

McClellan, S. L., and Franses, E. I., "Mechanisms of Competitive Adsorption of Albumin and Sodium Myristate at the Silicon Oxide/Aqueous Interface," *Langmuir*, 21, 10148-10153. (2005). 18th International Symposium on Chirality (ISCD-18), Busan, Korea, June 2006, "Direct Probing of Interactions of Solvents and Chiral Solutes with Amylose tris (3,5 dimethylphenylcarbonate) Sorbent," with R.B. Kasat, S.Y. Wee, H. W. Hillhouse, K. T. Thomson, and N.-H. L. Wang.

American Physical Society Annual Meeting, November 2005, "Measurements of Surface Properties with Oscillating Supported Bubbles," with Y.-C. Liao and O.A. Basarano.

AIChE Annual, Cincinnati, Ohio, November 2005, "Molecular Mechanisms of Selective Sorption of Chiral Enantiomers on Amylose-Based Sorbents;" with R.B. Kasat, K. Thomson, H.W. Hillhouse, and N.-H.L. Wang.

AIChE Annual, Cincinnati, Ohio, November 2005, "Physically Self -Assembled Monolayers (PSAM's) of Leicthin Lipids of Hydrophilic Silicon Oxide Interfaces."

AIChE Annual, Cincinnati, Ohio, November 2005. "Mechanisms of Competitive Adsorption of Albumin and Sodium Myristate at the Silicon Oxide/Aqueous Interface;" with S. J. McClellan.

AIChE Annual, Cincinnati, Ohio, November 2005, "Competitive Adsorption of Fibrinogen and Dipalmitoylphosphatidylcholine of Air/Aqueous Interface;" with S.K.Kim.



Robert E. Hanneman

M.D., Indiana University, 1959

Visiting Professor

Research Areas

Aerosols in medical practice, Surfactants in respiratory distress syndrome treatment, Non-invasive diagnostic techniques, Serum bilirubin determination by skin reflectance

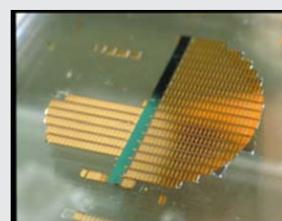
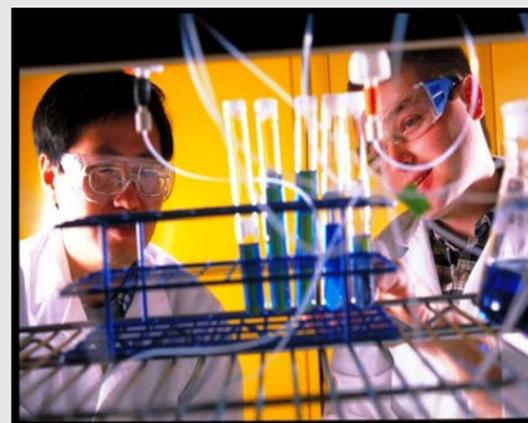
Selected Professional Activities

Indiana Chapter, American Academy of Pediatrics

Visiting Professor – Biomedical Engineering, Purdue University

Visiting Professor - Department of Child Psychology - Purdue University

Secretary's (Health and Human Services) Advisory Committee on Infant Mortality. Co-Chairman – Subcommittee on Low Birth Weight.



Michael T. Harris

Ph.D, University of Tennessee-Knoxville, 1992

Professor and Interim Associate Dean for Undergraduate Education

AICHE Grimes Award, 2005

Purdue Engineering Mentoring Award, 2006

Research Areas

Nanoparticle Technology, Synthesis of Nanowires and Nanotubes, Micropatterning, Protein Crystallization, Interfacial and Transport Phenomena

Selected Professional Activities

Member, Career and Education Operating Council-AICHE, 2005-06

Committee on Minority Affairs, American Chemical Society, 2006

Member, Minority Faculty Forum/Minority Affairs of AIChE 2005-2006

Chair Area 8d (Ceramics) of AIChE, 2005

Selected Invited Lectures

M. T. Harris, "USAXS and SAXS Studies of Nanostructured Materials and NanoParticles," National Society of Black Physicists/National Society of Hispanic Physicists, Orlando, Florida (Feb 16 – 19, 2005).

M. T. Harris, "Early Stage Nanoparticle Formation and the Coating of Nanoparticles on Biotemplates," Department of Chemical Engineering and Materials Science, University of Cincinnati; Cincinnati, Ohio (May 2005).

M. T. Harris, "Early Stage Nanoparticle Formation And Coating Or Nanoparticles On Biotemplates," Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, NJ (November 2005).



Selected Publications

S.Y. Lee, E. Royston, J. N. Culver and M. T. Harris, "Improved Metal Cluster Deposition on Genetically Engineered Tobacco Mosaic Virus Template," *Nanotechnology*, 16, S435-S441 (2005).

Y. Hyunmin, S. Nisar, S.Y. Lee, M. A. Powers, W. E. Bentley, G. F. Payne, R. Ghodssi, G. W. Rubloff, M. T. Harris, and J. N. Culver, "Patterned Assembly of a Genetically Modified Viral Nanotemplate via Nucleic Acid Hybridization," *NanoLetters*, 5(10), 1931-1936 (2005).

S.Y. Lee, and M. T. Harris, "Surface Modification of Maghemite Nanoparticles Capped by Oleic Acids: Characterization and Colloidal Stability in Polar Solvents," *J. Colloid Interface Sci.*, 293(2), 401-408 (2006).

S. Y. Lee, E. Royston, J. N. Culver and M. T. Harris, "Effect of the Concentration of CuCl₂ on the Aggregation and Mineralization of the Wild-type Tobacco Mosaic Virus Template," *J. Colloid Interface Sci.*, 297(2), 554-560 (2006).

J. Choi, E. Royston, D. Janes, J. N. Culver, and M. T. Harris, "Deposition of Platinum Clusters on the Surface Modified Tobacco Mosaic Virus," *J. Nanoscience and Nanotechnology*, 6(4), 974-981 (2006).

E. S. Royston, S. Y. Lee, J. N. Culver and M. T. Harris, "Characterization of Silica-Coated Tobacco Mosaic Virus," *J. of Colloid and Interface Science*, 298(2), 706-712 (2006).

Selected Conference Presentations

K. Srinivasan, S. Cular, V. R. Bhethanabotla, S. Y Lee, M. T. Harris, J. N. Culver, "Palladium Nanoparticle Coated Tobacco Mosaic Virus Sensing Layer Based Surface Acoustic Wave Hydrogen Sensor," TH002d, AIChE Annual Meeting, October 2005.

S. Y. Lee and M. T. Harris, "Surface Modification of Magnetic Nanoparticles: Characterization and Colloidal Stability in Polar Solvents," 08D05g, AIChE Annual Meeting, November 1, 2005.

E. S. Royston, J. N. Culver and M. T. Harris, "Silica Coating on a Bionanorod," 01C19c, AIChE Annual Meeting, November 1, 2005.

E. Widjaja and M. T. Harris, "A Fully Coupled Time Dependent 3-d Axisymmetric Simulation of an Evaporating Sessile Drop," 10D01b, AIChE Annual Meeting, October 31, 2005.

Y. Zhao, Y.Y. Won and M. T. Harris, "Calcium Alginate Gel Beads Synthesis by Electrodipersion in Vegetable Oils," 15015s, AIChE Annual Mtg, November 2, 2005.



Hugh W. Hillhouse

Ph.D., University of Massachusetts, 2000

Assistant Professor

Research Areas

Interfacial Engineering and Self-Assembly of Nanomaterials, Small-angle X-ray Scattering, Synthesis of Nanoporous, Thin Films, Electrochemistry of Nanoporous Films, Nanomaterials for Energy Conversion: Photovoltaics and Thermoelectrics

Selected Professional Activities

Symposium co-Organizer for 3 day symposium on "Synthesis, Characterization and Applications of Mesostructured Thin Layers." European Materials Research Society (E-MRS), Strasbourg France, June 2005.

Symposium co-Organizer, "Nucleation and Growth of Nanostructured Materials." ACS Annual Meeting, San Diego CA, March 2005.

Session Chair, "Thin Films and Functional Materials," Int'l Symposium on Zeolites and Microporous Materials (ZMPC), Japan, Aug., 2006

Session Chair, "Nanostructured Thin Films" AIChE Annual Mtg, San Francisco CA, 2006

Session Chair, "Self-assembly of Templated Inorganic Materials I," AIChE Annual Meeting, Cincinnati OH, 2005

Session Chair, "Nanostructured Thin Films" AIChE Annual Mtg, Cincinnati OH, 2005

Selected Invited Lectures

"Controlling Interfacial Curvature with Nanoclusters: A Robust Route to Fabricate Double Gyroid Thin Films out of Virtually Any Material," Nanoparticle Science & Engineering NSF IGERT Seminar Series, University of Minnesota, March 24, 2006.

"A New Class of Electrodes: Controlling Structure at the 5 nm Length Scale," Departmental Seminar, Chemistry Department, Carnegie Mellon University, Pittsburgh PA, March 9, 2006.

"Self-Assembled Nanostructured Films," Rohm and Haas Company, Spring House PA, September 22, 2006.

"Developing Nanostructured Thermoelectric Films," Lockheed Martin Corporation, Palmdale CA, June 16, 2006.

Selected Publications

Wei, T.C. & Hillhouse, H.W., "Ion Transport in the Microporous Titanosilicate ETS-10." *J. Phys. Chem. B* 110, 13728-13733 (2006).

Tate, M.P., Urade, V.N., Kowalski, J.D., Wei, T.C., Hamilton, B.D., Eggiman, B.W., & Hillhouse, H.W., "Simulation and Interpretation of 2D Diffraction Patterns from Self-Assembled Nanostructured Films at Arbitrary Angles of Incidence: from Grazing Incidence (above the critical angle) to Transmission Perpendicular to the Substrate," *J. Phys. Chem. B* 110, 9882-9892 (2006).

Eggiman, B.W., Tate, M.P., & Hillhouse, H.W., "Rhombohedral Structure of Highly Ordered and Oriented Self-Assembled Nanoporous Silica Thin Films," *Chem. Mater.* 18, 723-730 (2006).

Kasat, R.B., Zvinevich, Y., Hillhouse, H.W., Thomson, K.T., Wang, N.H.L., Franses, E.I., "Direct probing of sorbent-solvent interactions for amylose tris(3,5-dimethylphenylcarbamate) using infrared spectroscopy, X-ray diffraction, solid-state NMR, and DFT modeling," *J. Phys. Chem. B* 110, 14114-14122 (2006).

Tate, M.P., Eggiman, B.W., Kowalski J.D. & Hillhouse, H.W., "Order and Orientation Control of Mesoporous Silica Films on Conducting Gold Substrates Formed by Dip-Coating and Self-Assembly." Invited contribution to the Robert Rowel Special Issue of *Langmuir* 21, 10112-10118 (2005).

Urade, V.N., Hillhouse, H.W., "Synthesis of Thermally Stable Highly Ordered Orthorhombic Tin Oxide Thin Films." *J. Phys. Chem. B* 109, 10538-41 (2005).

Selected Conference Presentations

Hillhouse, H.W., "Electrochemistry and Nanofabrication with Mesoporous Silica Film Coated Electrodes." 5th Int'l Mesostructured Materials Symposium, Shanghai, PRC, Aug. 6, 2006.

Hillhouse, H.W., "Self-Assembly and Electrochemical Characterization of Highly Ordered and Oriented Mesoporous Silica Films." Int'l Symposium on Zeolites and Microporous Crystals, Yonago, Japan, Aug. 2, 2006.

"Using Grazing-angle-of-Incidence Small-Angle X-ray Scattering (GISAXS) to Characterize Nanoporous Films," Int'l Symposium on Zeolites and Microporous Crystals (ZMPC) Presymposium, Tokyo, Japan, 2006.

Tate, M.P., & Hillhouse, H.W. "GISAXS and FESEM as Tools to Investigate the Order and Orientation of Self-Assembled Mesoporous Silica Thin Films on Gold Substrates" AIChE Annual Meeting, Cincinnati OH, November 2005.

Urade, V.N., Hillhouse, H.W. "Investigations Into the Use of Organic Molecules as Probes for Determining the Pore Area and Accessibility in Titania Mesoporous Thin Films." AIChE Annual Meeting, Cincinnati OH, November 2005.

Wei, T.C. & Hillhouse, H.W. "Accessibility and Stability of Mesoporous Silica Thin Films Determined by Electrochemical Methods." AIChE Annual Meeting, Cincinnati OH, November 2005.



R. Neal Houze

Ph.D., University of Houston, 1968

Professor

Research Areas

Interphase mass transfer, Free boundary turbulence

Selected Professional Activities

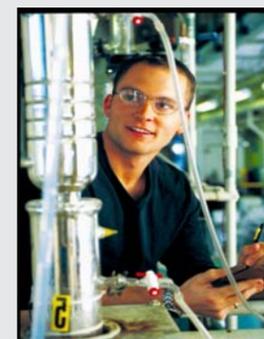
Coordinator, ABET Program in Chemical Engineering, 2006 - present

Panel Member, National Science Foundation, CCLI Program, August 2005

Coordinator, Cooperative Engineering Education Program in Chemical Engineering, 2005-present

Mediator, College of Engineering, 2005-present

Faculty Affiliate, Center For Instructional Excellence, Purdue University, 2004-present





Sangtae Kim

Ph.D Princeton, 1983

*Donald W. Feddersen Distinguished Professor
National Academy of Engineering*

Research Areas

Pharmaceutical informatics:
Bioinformatics, Cheminformatics, Systems Biology
Computational Microfluidics and Nanofluidics
Radio Frequency Identification (RFID)

Selected Professional Activities

Division Director, NSF Division, Shared Cyberinfrastructure (2005)
Consulting Editor (Information Technology), AIChE Journal
Chair, Awards Committee, SuperComputing06
Chair IT Subgroup, Food and Drug Administration Review Group
for Science and Technology

Selected Invited Lectures

“Fluidic Self Assembly and the Network of Things”:
Dept. of Chemical Engineering, SUNY Buffalo, Buffalo, NY, 2005
Dept. of Chemical Engineering, Univ. of Arizona, Tucson, AZ, 2006
Dept. of Chemical Engineering, UCSB, Santa Barbara, CA, 2006
Dept. of Industrial and Systems Engineering, OSU, Columbus, OH, 2006
Dept. of Chemical Engineering, Texas Tech, Lubbock, TX, 2006
“Cyberinfrastructure and Economic Curvature”: Eli Lilly and Company,
Indianapolis, IN, 2006
Initiative in Innovative Computing Program, Harvard University,
Cambridge,

Selected Publications

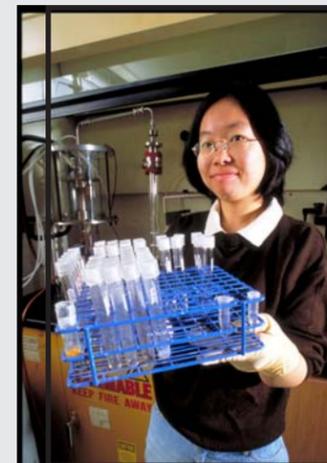
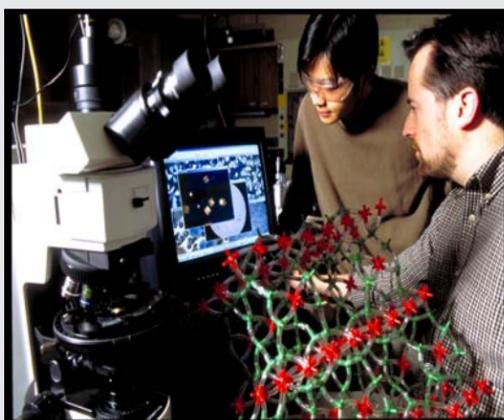
“Emerging Cyberinfrastructure: Challenges for the Chemical Process Community,” S. Kim and M. Heller, *Computers and Chemical Engineering* 30,1497-1501 (2006).
“Microhydrodynamics: Principles and Selected Applications,” DoverPublications (selected for reprint series by the Dover Editorial Board in recognition of “enduring value”).
Freeman, P.A., Crawford, D.L., Kim, S. and Munoz, J.L. (2005)
“Cyberinfrastructure for science and engineering: promises and challenges,” *Proc. of the IEEE* 93, 682-691.

Selected Conference Presentations

“A Position Specific Interaction Based Scoring Technique for Virtual Screening”, R.K. Nandigam, C. Chuaqui, J. Singh, Z. Deng, S. Kim, ACS Symposium, San Francisco, CA, 2006.
“Computational Approaches for Prediction of Cross Reactivity in Human Protein Kinome,” S. Maddipati, A. Fernandez and S. Kim, AIChE Annual Meeting, San Francisco, CA, 2006.
“Mediating Fluidic Self-Assembly with Optical Traps,” A.H. Ewing, S.Wereley and S. Kim, AIChE Annual Meeting, San Francisco, CA, 2006.

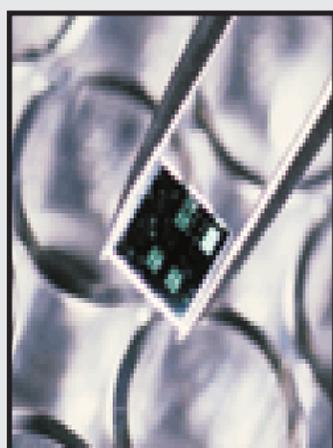
Named lectureships

Arnie G. Fredrickson Lecture (2006), Univ. of Minnesota
Benton Lecture (2005), Univ. of Florida
Barnett F. Dodge Lecture (2005), Yale University



Associated Engineering Facilities

Birck Nanotechnology Center



Just as antibiotics, the silicon transistor, and plastics affected nearly every aspect of society in the second half of the past century, nanoscale science, engineering, and technology will transform the 21st century. The *Birck Nanotechnology Center (BNC)* at Purdue University is a leading-edge national center advancing the frontiers of nanoscale research. The *Birck Nanotechnology Center* is housed in a new \$54 million state-of-the-art building constructed in Discovery Park on the western portion of the WL campus. This building is one of the most advanced facilities in the world, with specialized laboratories for nanoscale chemistry, physics, and biology; semiconductor-grade cleanrooms; and office space for faculty, post-docs, and graduate students from various disciplines across campus.



Gil Lee

Ph.D, University of Minnesota, 1992

Associate Professor

ETS Walton Fellow 2006-2007

Research Interests

Nanometer Scale Science in Medicine and Biotechnology,
Surface Forces in Macromolecular Systems, Ultrasensitive Biosensors

Selected Professional Activities

Co-Chair of the International Conference on Bioengineering and Nanotechnology,
Sept 3-7, 2006, Santa Barbara, CA.

AICHE Executive Board, National Planning Committee 2005

AICHE Executive Board, Programming Committee

AICHE Executive Board, Nanoscale Science and Engineering Forum

Selected Invited lectures

Synthesis and Characterization of High Uniformity Superparamagnetic
Microparticles, Meeting on Magnetic Separation and Nanomagnetism,
Karlsruhe, 4-5 Oct. 2006.

Application of Superparamagnetic Microparticles to Single
Molecule Measurements and Diagnostic Devices, U Florida, September 2006.

Novel Magnetic Materials for Diagnostic and Separation Applications,
DuPont Research Station, Delaware, March 2006.

Application of Magnetic Nanotechnology to Diagnostic Devices,
Pennsylvania State University, March 2006.

Study of Aplysia Californica with AFM, Trinity Univ, Dublin, Ireland, 2005.

Selected Publications

E.L. Grzywa, A.C. Lee, G.U Lee, and D. Suter, Comparative Atomic Force
and Optical Microscopy Study of Neuronal Growth Cones, in press *J.
Neurobiology* 2006.

Z. Wang, H. Shang, and G.U Lee, Nanoliter Scale Reactor Arrays for
Biochemical Sensing, 22, 6273-6276, *Langmuir* 2006.

J.-W. Park and G.U Lee, Properties of Mixed Lipid Monolayers Assembled on
Hydrophobic Surfaces through Vesicle Adsorption, *Langmuir* 22:5057-5063,
2006.

Shang, H., W. S. Chang, S. H. Kan, S. A. Majetich and G. U. Lee, Synthesis
and Characterization of Paramagnetic Microparticles Through Emulsion
Templated Free Radical Initiated Polymerization. *Langmuir* 22:2516-2522,
2006.

Z.G. Wang, R.T. Haasch, and G.U Lee, A Mesoporous Membrane Device for
Assymmetric Biosensing, *Langmuir* 21, 1153-1157, 2005.

H. Shang and G.U Lee, Magnetic Tweezers: A Powerful Tool for
Highthroughput Screening of Peptide Libraries, *Magnetism and Magnetic
Materials* 293, 382-388, 2005.

Selected Conference Presentations

G.U Lee, D.M. Suter, A. Lee, Y. Xiong, E.L.Grzywa, and, "Comparative
Atomic Force and Optical Microscopy Study of Neuronal Growth Cone
Morphology," International Conference on Nanoscience and Technology 2006,
July 2006, Basel, Switzerland.

H. Shang and G.U Lee, "The Application of Magnetic Tweezers to High
Throughput Screening of Peptide Libraries," Annual Meeting of the AVS, Nov.
2005, Boston, MA.

K.J. Jeong, S. Bhattacharya, D.B. Janes, and G.U Lee, "Design Rules for the
Assembly of DNA Modified Nanoparticles: Influence of Surface Chemistry,
Ionic Strength, and a Polycation," Annual Meeting of the AVS, Nov. 2005,
Boston, MA.

A.K. Mahapatro, K.J. Jeong, S. Ghosh, S. Bhattacharya, G. Lee, and D.
Janes, "Measurement of Single Molecule Conductance with Nanoscale Break
Junctions," Annual Meeting of the AVS, Nov. 2005, Boston, MA.

W. S. Chang, T.D. Sands, and Gil U Lee, "Synthesis and Characterization
of AuFe Alloy Magnetic Nanoparticles," Annual Meeting of the AICHE, Nov.
2005, Cincinnati, OH.

Emilie L. Grzywa, A. C. Lee, and D. Suter, G.U Lee, "A Study of Structure of
Aplysia californica Neuron Growth Cones using Atomic Force and
Epifluorescence Microscopy, " Annual Meeting of the AICHE, Nov. 2005,
Cincinnati, OH.



Julie C. Liu

Ph.D, CalTech, 2006

Assistant Professor

Whitaker Foundation Fellowship in Biomedical Engineering

Dr. Liu will be joining the School in January 2008

Research Interests

Biomaterials, Tissue Engineering, Protein Engineering

Associated Engineering Facilities

Bindley Bioscience Center



The *Bindley Bioscience Center* initiates and facilitates multi-investigator, multi-disciplinary research that blends life sciences and engineering. State-of-the-art research programs focus along strategic lines that advance proteomic science and technology, bionanotechnology and biomicrotechnology, spectroscopy-microscopy for cellular and tissue imaging, tissue engineering, and bio-informatics. Researchers in the Center already are at work designing tiny electronic devices that use proteins, DNA, and even living cells to rapidly detect substances in blood, air, water and food, leading the way for innovative and rapid diagnostic tools. Proteomics and cellular imaging are opening future opportunities in tissue engineering - creating materials that can mimic, repair and regenerate biological tissues and promote self-healing. These and other exciting advancements and discoveries will shape our future. We encourage your collaboration and participation as we work together to merge engineering and the life sciences in new and productive ways.



John A. Morgan

Ph.D., Rice, 1999

*Associate Professor
Director, Undergraduate Studies*

Research Areas

Metabolic Engineering, Biocatalysis

Selected Professional Activities

Associate Editor "Bioprocess and Biosystems Engineering"

Selected Invited lectures

Theoretical and Experimental Approaches to the Autotrophic Metabolic Flux Characterization, Plant Biology Department, Michigan State University, February 2005.

Engineering of flavonoid biosynthesis in yeast. Chemical Engineering Department, Rice University, October 2005.

Metabolic engineering of plant pathways in yeast. Biomedical Engineering Department, University of Utah, October 2005.

Engineering of plant metabolism. Chemical Engineering, Rensselaer Polytechnic Institute, January 2006

Selected Publications

Shastri, A. and Morgan, J.A. (2005) Flux Balance Analysis of Photoautotrophic Metabolism (accepted *Biotech. Prog.* **21**, 1617-26).

Chen, H. and Morgan, J.A. (2005) High throughput screening of heterologous P450 whole cell activity (*Enzyme & Microbial Tech.*, in press).

Jiang, H. and Morgan, J.A. (2005) Metabolic Engineering of the Phenylpropanoid Pathway in *Saccharomyces cerevisiae*, *Appl. Environ. Microbiol.* **71**, 2962-2969.

Selected Conference Presentations

Jiang, H. and Morgan, J.A., "Metabolic engineering of the phenylpropanoid pathway for the synthesis of flavonoids." Biochemical Engineering XIV, Harrison Hot Springs, Canada, July 2005.

Shastri, A. and Morgan, J.A., "Flux balance analysis of photoautotrophic metabolism." Biochemical Engineering XIV, Harrison Hot Springs, Canada, July 2005.

LaClair, C.E., Morgan, J.A., "A novel technique to measure yeast generational lifespan." ACS National Meeting, San Diego, March 2005.

Morgan, J.A. Chen, H., Jiang, H. Engineering of flavonoid biosynthesis in yeast. Natural Products Discovery and Production. New challenges, new opportunities. Santa Fe, NM. June 2006.



Joseph F. Pekny

Ph.D., Carnegie Mellon University, 1989

Professor

Director, e-Enterprise Center at Discovery Park
Founding Director, Regenstrief Center for
Healthcare Engineering*

Research Areas

Systems analysis, combinatorial optimization, supply chain management, planning and scheduling systems, pharmaceutical pipeline management, model-based and data driven management, systems analysis and decision models in healthcare engineering, and real-time decision systems

Selected Professional Activities

Advisory Board Member, Center for Implementing Evidence-Based Practice, Roudebush Veterans Administration Medical Center, Indianapolis, Indiana

Selected Invited Lectures

"The Role of Healthcare Engineering in the Indiana Patient Safety Center," Indiana Council of Quality and Patient Safety, Indianapolis, Indiana, March 2006.

"An Overview of Research and Applications in Healthcare Engineering," Indiana Association for Healthcare Quality, Indianapolis, Indiana, April 2006.

"Future Possibilities in Cancer Care Based on Engineered Systems," Saint Vincent Health Research Symposium, Indianapolis, Indiana, May 2006.

"A Simulation Optimization Based Architecture for Robust R&D Project Portfolio and Resource Management," Air Products and Chemicals Seminar, May 2006.

"Engineering an Ever Improving System for Cancer Care: The Indiana Living Laboratory," Joint Indiana University-Purdue University Conference on Cancer Care Engineering, Lebanon, Indiana, June 2006.

Selected Publications

Aydogan, S., Orcun, S., Blau, G., Pekny, J. F., and G.V. Reklaitis, (2005) "Determining Optimum Planting Schedule Using Diet Optimization and Advanced Crop Scheduling Models," Proceedings of the 35th International Conference on Environmental Systems (ICES), 11-14 July 2005, Rome, Italy, SAE Technical Paper 2005-01-2815.

Aydogan, S., Orcun, S., and J. F. Pekny, "Effect of Different Waste Recovery Systems on the Overall Waste Generation Rates for an Advanced Life Support System," International Journal of Environment and Pollution, (Accepted).

Varma, V., G. E. Blau, J. F. Pekny, and G. V. Reklaitis, "A Framework for addressing Stochastic and Combinatorial aspects of Scheduling and Resource Allocation in Pharmaceutical R&D Pipelines," Special Issue of Computer and Chemical Engineering (invited).

Selected Conference Presentations

Aydogan S., S. Orcun, G. Blau, J. F. Pekny and G. V. Reklaitis, "Life Support System Design Characterization using SIMOPT," Presentation at Habitation Conference, February 5-8 2006, Orlando, FL.

Aydogan, S., S. Orcun, G. Blau, J. F. Pekny, and G.V. Reklaitis, "A Simulation-Based Optimization Approach to the Evolution of an Advanced Life Support System for Mars Base," Presented at the American Institute of Chemical Engineers (AIChE) Annual Meeting, 30 October - 4 November 2005, Cincinnati, OH.

Daichendt, M. M., A. Esmaili, D. Schertz, J. F. Pekny, "Exploring New Business Opportunities through an Innovative Collaboration between Industry and Academia: Leveraging Advances in Optimization with a Market Model for Cap & Trade Emissions," Presented at the American Institute of Chemical Engineers (AIChE) Annual Meeting, 30 October - 4 November 2005, Cincinnati, OH.

*e-Enterprise Center



The *e-Enterprise Center* initiates and pulls together a myriad of related new-technology activities on the Purdue University campus, with a special focus on three core areas where Purdue has, or can develop, national leadership: (1) Network security and reliability; (2) Management of distributed e-enterprise, including database systems, and (3) Logistics and distribution of products and marketing of e-Enterprise. The e-Enterprise Center brings together faculty and students with strengths in database systems design and integration engineering, software engineering, communication, management, operations systems, production systems, decision theory applications, system performance, risk evaluation, marketing, customer service and model simulation. Through this center, an entire business - commerce, supply chain, management, operations, product life-cycle control, customer service and data security - can be modeled, analyzed and made more efficient. Working with Purdue's industrial and government partners, the center is an interactive test bed, which combines computer models with human behavior at various levels (from strategy formulation to operations management) in a real-world environment.



R. Byron Pipes

Ph.D., University of Texas at Arlington, 1972

*John Leighton Bray Distinguished Professor of Engineering
National Academy of Engineering*

Research Areas

Application of nanotechnology to engineering disciplines including aerospace, composite materials and polymer science and engineering.

Selected Professional Activities

Editorial Boards

Composites Science and Technology, Elsevier Publishers
Journal of Composite Materials, Sage Publications
Composite Structures, Elsevier Publishers

Selected Invited lectures

Vanderbilt University, "Carbon Nanotechnology," Nashville, TN, February, 2006.

Spirit Aerosystems, "Polyimide Foams for Acoustic Applications," Wichita, KS, March, 2006.

University of Leoben, "van der Waals Interactions in Carbon Nanotubes," Leoben, Austria, July, 2006.



Selected Publications

Pipes, R.B. and Zalamea, L., "Energetics of Imperfectly Bonded Carbon Nanotube Arrays in Flexure," in press, *Composites Science and Technology*, 2006.

Salvetat, J-P, Bhattacharyya, S., and Pipes, R.B., "Progress on Mechanics of Carbon Nanotubes and Derived Materials," in press, *Journal of Nanoscience and Nanotechnology*, 2006.

C. I. Cano, E. S. Weiser, T. Kyu and R. B. Pipes, "Polyimide Foams from Powder: Experimental Analysis of Competitive Diffusion Phenomena," *Polymer*, 46(22), 2005, pp. 9296-9303.

Coffin D.W., Carlsson, L.A. and Pipes, R.B., "On the Separation of Carbon Nanotubes," in press, *Composites Science and Technology*, 2006.

Pipes, R.B., Hubert, Salvétat, J.-P. and Zalamea, L., "Flexural Deformation of the CNT Array as a Measure of van der Waals Interaction Forces," in press, *Composites Science and Technology*, 2006.

T.E. Chang, L.R. Jensen, A. Kisliuk, R.B. Pipes, R. Pyrz, A.P. Sokolov "Microscopic Mechanism of Reinforcement in Single-Wall Carbon Nanotube/Polypropylene Nanocomposite," *Polymer*, 46, 2005, pp 439-44

Selected Conference Presentations

American Society for Composites Conference, Dearborn Michigan, September 17-19, 2006.

US-Japan Conference on Composite Materials, Dearborn, Michigan, September 19-21, 2006.

2006 ASME International Mechanical Engineering Congress, November 5-10, 2006, Chicago, IL.

Foams 2006, Society of Plastics Engineering, Chicago, IL, September, 2006



Doraiswami Ramkrishna

Ph.D., University of Minnesota, 1965

*H. C. Peffer Distinguished Professor
Associate Head, School of Chemical Engineering*

Research Areas

Applied mathematics, Dispersed phase systems, Biochemical engineering, Chemical reaction engineering

Selected Professional Activities

Editorial Boards

*Iterational Journal of Applied Engineering Research
The World Journal of Chemical Engineering*

Member, Scientific Committee for Population Balance Conference Series.
Hawaii, USA (2000); Valencia, Spain (2004); Quebec, Canada (2007).

Member, Technology Advisory Board to General Mills, 2005.

Selected Invited lectures

Thomas Baron Award Lecture: "Population Balances. Future Prospects," A.I.Ch.E. Annual Meeting, November 10, 2005.

Department of Chemical Engineering, University of California at Los Angeles. "On Modeling Metabolic Systems. The Cybernetic Approach," March 11, 2005.

Department of Chemical Engineering, Washington University at St. Louis. "On Modeling Metabolic Systems. The Cybernetic Approach," April 25, 2005.

Indiana University Biocomplexity Workshop: "On Modeling Metabolic Systems. The Cybernetic Approach," May 9-12, 2005.

Amrita Institute of Medical Sciences, Cochin. "The Potential of Mathematical Models in Cancer Treatment," June 30, 2006.

Department of Chemical Engineering, Indian Institute of Technology, Chennai. "On Modeling Metabolic Systems. The Cybernetic Approach," July 10, 2006.

Selected Publications

Namjoshi, A. and D. Ramkrishna, "A Cybernetic Modeling Framework for Analysis of Metabolic Systems," *Computers and Chemical Engineering*, 29, 487-498, 2005.

Nere, Nandkishor and D. Ramkrishna, "Evolution of Drop Size Distributions in Fully Developed Turbulent Pipe Flow of a Liquid-Liquid Dispersion by Breakage," *Ind. Eng. Chem.*, (Wasan issue), 44, 1187-1193, 2005.

Qiang Qin, and D. Ramkrishna "The Effect of Operating Conditions on the Dispersion State of Supported Metal Catalysts: A Model Study," *Ind. Eng. Chem. Res.* (Dudukovic issue), 44, 6466-6476, 2005.

Nere, Nandkishor and D. Ramkrishna, "Solution of population balance equation with pure aggregation in a fully developed turbulent pipe flow," *Chem.Eng.Sci.* 61, 96-103, 2006.

Sherer, E., Rundell, A. E., Robinson, J. P., R. E. Hannemann and D. Ramkrishna, "Analysis of Resonant Chemotherapy in Leukemia Treatment via Multi-Stage Population Balance Models," *J. Theoretical Biol.*, 240, 648-661, 2006.

Young, J. D. and D. Ramkrishna, "On the Matching and Proportional Laws of Cybernetic Models," *Biotechnology Progress*, in press.

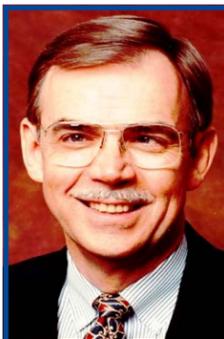
Selected Conference Presentations

Sherer, E., D. Ramkrishna, R. E. Hannemann and A. E. Rundell, "Evaluation of Leukemia Patient Non-Compliance During Maintenance Chemotherapy. A Population Balance Model of RBC Maturation," Paper 432a, A.I.Ch.E. Annual Meeting, 2005, Cincinnati, October 31-November 4, 2005.

Young, J. D. and D. Ramkrishna, "Discovery and Analysis of Biological Control Laws," Paper #379b, AIChE Annual Meeting, 2005, Cincinnati, October 31-November 4, 2005.

Young, J. D. and D. Ramkrishna, "Cybernetic Modeling Approach for Analysis and Redesign of Biochemical Pathways," Paper #479b, AIChE Annual Meeting, 2005, Cincinnati, October 31-November 4, 2005.

Young, J. D. and D. Ramkrishna, "Elementary Modes and Cybernetic Mechanisms: A Systems Level Approach for Modeling Biological Regulation," Paper #504a, A.I.Ch.E. Annual Meeting, 2005, Cincinnati, October 31-November 4, 2005.



Gintaras V. "Rex" Reklaitis

Ph.D., Stanford University, 1969

Edward W. Comings Professor of Chemical Engineering

Pharmaceutical Technology & Education Center, Co-director
NSF ERC on Structured Organic Composites, Deputy Director

Research Areas

Process Systems Engineering, Computer Aided Process Operations, Batch Process Design, Scheduling and Analysis

Selected Professional Activities

Editor-in-Chief, *Computers & Chemical Engineering*
Editorial Board, *Computer Applications in Engineering Education*
Editorial Board, *Journal of Pharmaceutical Innovation*

Selected Invited Lectures

"Enterprise-wide Decision Support Systems: PSE Contributions and Promise," European Symposium on Computer Aided Process Engineering -15, Barcelona, Spain, May 2005 (keynote).

"New Product Development Pipeline Management," Pan American Advanced Studies Institute on Process Systems Engineering, Iguazu Falls, Argentina, August 16-23, 2005 (Invited lecture series).

"Enterprise-wide Perspectives in Engineering Decisions," Merck Sharp & Dohme Lecture, Department of Chemical Engineering, University of Puerto Rico, Mayaguez, Oct 20, 2005.

"Decision Support for Pharmaceutical Product Pipeline Management," 12th Chemical Engineering Symposium, Department of Chemical Engineering, University of Puerto Rico, Mayaguez, Oct 21, 2005, (keynote).

Selected Publications

Wan, X, J.F. Pekny, and G.V. Reklaitis, "Simulation-based Optimization with Surrogate Models – Application to Supply Chains," *Computers & Chem Engr*, 29, 1317-1328, 2005.

Kuriyan, K., W. Muench, and G.V. Reklaitis, "The Dow Chemical Project: Creating a Web-based Interface to a Dynamic Simulation," *Comp. Appl. Engr. Ed.*, 13 250-256, 2006.

Yi, G. and G.V. Reklaitis, "Optimal Design of Batch-Storage Network for Multi-tasking Semicontinuous Processes," *AIChE J*, 52, 269-81, '06

Varma, V.A., G.E. Blau, J.F. Pekny and G.V. Reklaitis, "Enterprise-wide Modeling and Optimization: An Overview of Emerging Research Challenges and Opportunities," special issue *Computers & Chem Engr*, 30, 2006 (in press).

Selected Conference Presentations

"Pharmaceutical Informatics: A Novel Paradigm for Pharmaceutical Product Development and Manufacture," 15th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, May, 2005

"A Holistic Approach for Modeling Information and Knowledge in Development and Operations of Chemical Processes," paper 27a, AIChE Annual Meeting, Cincinnati, Ohio, October 2005

"An Informatics Framework for Pharmaceutical Product Development," paper 76c, AIChE Annual Meeting, Cincinnati, OH, Oct. 2005.

"From Discovery to Manufacturing Recipe Life Cycle Management," paper 104ea, AIChE Annual Meeting, Cincinnati, Ohio, October 2005.

"Optimal Design of Batch Storage Network under Random Failures and Waste Treatment Processes," paper 240w, AIChE Annual Meeting, Cincinnati, Ohio, October 2005.

"Systematic Modeling of Knowledge in Pharmaceutical Product Formulation," paper 437b, AIChE Annual Meeting, Cincinnati, Ohio, Oct. 2005.



Fabio H. Ribeiro

Ph.D., Stanford University, 1989

Professor

New York Catalysis Society Excellence in Catalysis Award, 2005

Research Areas

Surface Science and Kinetics of Heterogeneous Catalytic Reactions

Selected Professional Activities

Editorial Board for Applied Catalysis B: Environmental
Editorial Board for Catalysis Letters
Director, Catalysis and Reaction Engineering Division AIChE (2005-2008)
Member, Scientific Committee-19th North American Catalysis Society Meeting, May 2005, Philadelphia, PA. Chair, Novel Reaction Engineering session.
Organizer, Symposium on Nanoparticles, Colloids, and Surfaces in Advanced Catalytic Materials., 79th Annual American Chemical Society, Colloid and Surface Science Symposium, June 2005, Clarkson University.
Member, Proposal Review Committee, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Selected Invited Lectures

"A discussion of recent methodologies to study heterogeneous catalysis," Department of Chemical Engineering, University of Virginia, October 13, 2005.

"A discussion of recent methodologies to study heterogeneous catalysis," Department of Chemical Engineering, University of Michigan, October 27, 2005.

"A discussion of recent methodologies to study heterogeneous catalysis," Department of Chemical Engineering, University of Notre Dame, November 15, 2005.

"A discussion of recent methodologies to study heterogeneous catalysis," Department of Chemical Engineering, Brigham Young University, March 16, 2005.

"What is catalysis and how it is improving our environment?" Oak Ridge Chapter of ASM International, Educational Symposium on Heterogeneous Catalysis, Invited Talk, 4 April 2006, Oak Ridge, TN.

Selected Publications

"Temperature Dependence of Reaction Kinetics for Complete Oxidation of Methane on Palladium and Palladium Oxide," G. Zhu, J. Han, D. Yu. Zemlyanov, F. H. Ribeiro, *Physical Chemistry B*, 109, 2331-2337, 2005.

"NO₂ inhibits catalytic reaction of NO and O₂ over Pt," S.S. Mulla, N. Chen, W. N. Delgass, W. S. Epling, F. H. Ribeiro, *Catalysis Letters*, 100, 267-270, 2005.

"Effect of Potassium and water vapor on catalytic reaction of nitric oxide and dioxygen over platinum," S.S. Mulla, N. Chen, L. Cumarantunge, W. N. Delgass, W. S. Epling, F. H. Ribeiro, *Catalysis Today*, 114, 57-63, 2006.

"Interaction of O₂ with Pd Single Crystals in the range 1-150 Torr: Oxygen Dissolution and Reaction," J. Han, D. Y. Zemlyanov, and F. H. Ribeiro, *Surface Science*, 600, 2752-2761, 2006.

"Interaction of O₂ with Pd Single Crystals in the range 1-150 Torr: Surface Morphology Transformations," J. Han, D.Y. Zemlyanov, and F. H. Ribeiro, *Surface Science*, 600, 2730-2744, 2006.

"Reaction of NO and O₂ to NO₂ on Pt: Kinetics and Catalyst Deactivation," S. S. Mulla, N. Chen, L. Cumarantunge, G. E. Blau, D. Y. Zemlyanov, W. N. Delgass, W. S. Epling, F. H. Ribeiro, *Journal of Catalysis*, 241, 389-399, 2006.

Selected Conference Presentations

Shadab M., N. Chen, J. Ratts, L. Cumarantunge, W. Epling, W.N. Delgass, and F. Ribeiro, "NO Oxidation Reaction Kinetics over Pt/Al₂O₃ and Pt/K/Al₂O₃ Catalysts," 79th Annual ACS, Colloid and Surface Science Symp., June 12-15, 2005, Clarkson University, Potsdam, NY.

G. Zhu, J. Han, D. Zemlyanov, F.H. Ribeiro, "Reaction Kinetics and Structure Insensitivity of Catalytic Combustion on Palladium Catalysts," 6th Int'l Workshop on Catalytic Combustion, September 13, 2005, Island of Ischia, Italy.

F. H. Ribeiro, S. S. Mulla, N. Chen, L. Cumarantunge, B. R. Kromer, L. Cao, W. N. Delgass, J. M. Caruthers, and W. S. Epling, "Trapping of NO_x on Pt/Ba/Al₂O₃ using simulated diesel exhausts," Honoring ACS Somorjai Award Winner J. Dumesic, 30 March 2006, Div Colloid and Surface Chemistry, 231st ACS National Meeting, Atlanta, GA.



Kendall T. Thomson

Ph.D., University of Minnesota, 1999

Associate Professor

Research Areas

Computational Catalysis & Nanoporous Materials, Ab Initio Molecular Dynamics, Molecular Simulation & Modeling, Catalyst Design and Informatics

Selected Professional Activities

AIChE Catalysis & Reaction Engineering Div. Programming Vice Chair, '05-06
AIChE Catalysis & Reaction Engineering Div. Programming Chair, '06-present

Selected Invited lectures

"Towards Design of Novel Catalytic Materials Using Computational Chemistry," Georgia Tech, September 2005.

"Insights into Catalytic Activity Using Density Functional Theory," New York Catalysis Society, January 2006.

Selected Publications

T. A. Manz, A. E. Fenwick, K. Phomphrai, I. P. Rothwell, K. T. Thomson, "The Nature of Aryloxide and Arylsulfide Ligand Bonding in Dimethyltitanium Complexes Containing Cyclopentadienyl Ligation," *Dalton Transactions*, (4), 668-674 (2005).

Y. Joshi, K. T. Thomson, "Embedded Cluster (QM/MM) Investigation of C6 Diene Cyclization in H-ZSM-5," *J. of Catalysis*, 230, 440-463 (2005).

Y. Joshi, K. T. Thomson, "The Roles of Gallium Hydride and Brønsted Acidity in Light Alkane Dehydrogenation Mechanisms using Ga Exchanged HZSM-5 Catalysts: A DFT Pathway Analysis (INVITED PAPER)," *Catalysis Today*, 105, 106-121 (2005).

A. Deskins, J. Lauterbach, K. T. Thomson, "Lifting the Pt{100} Surface Reconstruction Through Oxygen Adsorption: A DFT Analysis," *J. of Chemical Physics*, 122, Art. No. 184709 (2005).

A. Joshi, W. N. Delgass, K. T. Thomson, "A Comparison of the Catalytic Activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in the Gas-Phase Reaction of H₂ and O₂ to Form Hydrogen Peroxide: A DFT Investigation," *J. of Physical Chemistry B*, 109, 22392-22406 (2005).

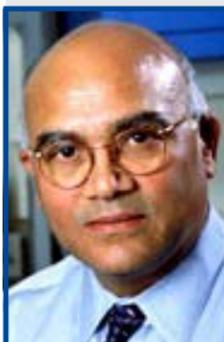
A. Joshi, W. N. Delgass, K. T. Thomson, "Partial Oxidation of Propylene to Propylene Oxide over a Neutral Gold Trimer in the Gas Phase: A DFT Study," *J. of Physical Chemistry B*, in press (2006).

Selected Conference Presentations

K.T. Thomson and Y. Joshi, "The Roles of Gallium Oxide and Brønsted Acidity in Light Alkane Dehydrogenation Using Ga-HZSM-5," 19th NAM of the North American Catalysis Society, Philadelphia, 2005.

Charles L. Schaffer and Kendall T. Thomson, "Density Functional Theory Investigation of the Hydrolysis and Condensation of Polysilicic Acid: a Mechanistic and Energetic Analysis," AIChE Annual Meeting, Cincinnati, 2005.

Ajay M. Joshi, W. Nicholas Delgass, and Kendall T. Thomson, "Hydrogen Peroxide Formation and Propylene Epoxidation on Gas-Phase Au Clusters," AIChE Annual Meeting, Cincinnati, 2005.



Arvind Varma

PhD., Minnesota, 1972

R. Games Slayter Distinguished Professor and Head, School of Chemical Engineering

Technology and Innovation Award, *Industry Week*, 2005

Research Areas

Heterogeneous Combustion, Hydrogen and other Energy Sources, Chemical and Catalytic Reaction Engineering

Selected Professional Activities

Series Editor, *Cambridge Series in Chemical Engineering*, Cambridge University Press

Editorial Board, *International Journal of Self-Propagating High-Temperature Synthesis*

Board of Directors, ISCRE, Inc.

Member, Scientific Committee, ISCRE-19, Potsdam/Berlin, Germany, Sept. 2006

Chair, Sessions (2) in honor of Neal Amundson's 90th Birthday, 2006
AIChE Annual Meeting, San Francisco, CA.

Chair, Sessions (2) in honor of Wilhelm Award Recipient, 2006
AIChE Annual Meeting, San Francisco, CA.

Selected Invited lectures

University of California, Los Angeles, CA, February 2005

CPE-Lyon, Lyon, France, June 2005

Politecnico di Milano, Milano, Italy, June 2005

Drexel University, Philadelphia, PA, May 2006



Selected Publications

"Combustion of Novel Chemical Mixtures for Hydrogen Generation," E. Shafirovich, V. Diakov and A. Varma, *Combustion and Flame*, 144, 415-418 (2006).

"A Numerical Study of Combustion Stability in Emergency Oxygen Generators," V. Diakov, E. Shafirovich, A. Varma, *AIChE Journal*, 52, 1495-1501 (2006).

"Single and Multi-Wall Carbon Nanotubes by Floating Catalyst Method: Synthesis, Purification and Hydrogen-uptake Measurements," Y.-Y. Fan, A. Kaufmann, A. Mukasyan and A. Varma, *Carbon*, 44, 2160-2170 (2006).

"Novel Perovskite-Based Catalysts for Autothermal JP-8 Fuel Reforming," P. Erri, P. Dinka and A. Varma, *Chem. Engr. Science*, 61, 5328-5333 (2006).

"Heterogeneous Combustion: Recent Developments and New Opportunities for Chemical Engineers," A. Varma, V. Diakov and E. Shafirovich, *Perspective Article, AIChE Journal*, 51, 2876-2884 (2005).

"Review: Influence of Gravity on Combustion Synthesis of Advanced Materials," A. S. Mukasyan, C. Lau and A. Varma, *AIAA Journal* 43, 225-246 (2005).

Selected Conference Presentations

"Hydrogen Generation via Combustion of Metal Borohydride/Aluminum/Water Mixtures," ACS National Meeting, Washington, DC, August 2005.

"Novel Chemical Mixtures for Hydrogen Generation by Combustion," AIChE Annual Meeting, Cincinnati, OH, November 2005.

"Numerical Modeling of Combustion Stability in Emergency Oxygen Generators," AIChE Annual Meeting, Cincinnati, OH, November 2005.

"Studies on Ignition and Combustion Mechanisms of Single Ni-Coated Al Particles," 44th AIAA Aerospace Sciences Meeting, Reno, NV, January 2006.

"Combustion-Based Methods to Generate Hydrogen for Fuel Cells," NSF Workshop on *Research Frontiers for Combustion in the Hydrogen Economy*, Arlington, VA, March 2006.

"Solution Combustion Synthesized Oxygen Carriers for Chemical Looping Combustion," ISCRE-19, Potsdam, Germany, September 2006.



Venkat Venkatasubramanian

PhD, Cornell, 1984

Professor

Shreve Award for Outstanding Teaching, 2006

Omega Chi Mentoring Award, 2005

Teaching for Tomorrow Award, 2005

Research Areas

Pharmaceutical Informatics, Abnormal Events Management and Process Safety, Discovery Informatics for Molecular Products Design, Systems Biology, Complex Adaptive Systems, Artificial Intelligence, Artificial Life, and Statistical Mechanics.

Selected Professional Activities

Member of the Editorial Board, Computers and Chemical Engineering, 2000-Present

Academic Trustee, Computer Aids in Chemical Engineering Corporation (CACHE Corp.), Austin, TX, 1993-present.

Selected Invited Lectures

Plenary Speaker, International Conference on Chemical Process Control CPC 7, Lake Louise, Alberta, Canada, Jan 2006.

Selected Publications

Zhao, C., Bushan, M. and V. Venkatasubramanian, "PHASuite: An Automated HAZOP Analysis Tool for Chemical Processes Part I Knowledge Engineering Framework," in press, *Process Safety and Environmental Protection, Trans IChemE Part B*, 83 (B6), 2005.

Zhao, C., Bushan, M. and V. Venkatasubramanian, "PHASuite: An Automated HAZOP Analysis Tool for Chemical Processes Part II. Implementation and Case Study," in press, *Process Safety and Environmental Protection, Trans IChemE Part B*, 83 (B6), 2005.

Venkatasubramanian, V., Politis, D. N., and Patkar, P. R., "Entropy Maximization as a Holistic Design Principle for Complex Optimal Networks," in press, *AIChE J*, 52(3), 2006.

Maurya, M. R., R. Rengaswamy and V. Venkatasubramanian, "A Signed Directed Graph-Based Systematic Framework for Steady-State Malfunction Diagnosis Inside Control Loops," in press, *Chem. Engg. Sci.*, 61, 2006, pp. 1790-1810.

Maurya, M. R., Katare, S. R., Patkar, P. R., Rundell, A. E., and Venkatasubramanian, V., "A Systematic Framework for the Design of Reduced-order Models for Signal Transduction Pathways from a Control Theoretic Perspective," in press, *Comp. Chem. Engg.*, 2006.

Maurya, M. R., Bornheimer, S. J., Venkatasubramanian, V. and Subramanian, S., "Reduced-Order Modeling of Biochemical Networks: Application to the GTPase- Cycle Signaling Module," in press, *IEE Systems Biology*, 2006.

Selected Conference Presentations

C. Zhao, G. Joglekar, A. Jain, V. Venkatasubramanian, G. V. Reklaitis, "A Holistic Approach for Modeling Information and Knowledge in Development and Operations of Chemical Processes," paper 27a, AIChE Annual Meeting, Cincinnati, OH, 2005.

C. Zhao, A. Jain, L. M. Hailemariam, G. Joglekar, V. Venkatasubramanian, G. V. Reklaitis, K. R. Morris, A. Hlinak, P. K. Basu, "An Informatics Framework for Pharmaceutical Product Development," paper 76c, AIChE Annual Meeting, Cincinnati, OH, 2005.

A. Giridhar, B. B. Krishnamurthy, R. Agrawal, V. Venkatasubramanian, "Particle Swarm Optimization in Discontinuous Function Spaces," paper 106a, AIChE Annual Meeting, Cincinnati, OH, 2005.

S. H. Hsu, G. E. Blau, J. M. Caruthers, W. N. Delgass, F. H. Ribero, V. Venkatasubramanian, "A Statistical Methodology for Building Catalytic Reaction Models with High Throughput Experimentation," paper 114c, AIChE Annual Meeting, Cincinnati, OH, 2005.

G. Joglekar, C. Zhao, V. Venkatasubramanian, G. V. Reklaitis, "From Discovery to Manufacturing: Recipe Life Cycle Management," paper 104e, AIChE Annual Meeting, Cincinnati, OH, 2005.

J. M. Caruthers, W. N. Delgass, M. Abu-Omar, K. T. Thomson, V. Venkatasubramanian, G. E. Blau, T. A. Manz, G. Medvedev, J. Haq, K. A. Novstrup, K. Phomphrai, S. Sharma, B. B. Krishnamurthy, "Discovery Informatics for Catalyst Design: Single Site Olefin Polymerization Catalysts," paper 114g, AIChE Annual Meeting, Cincinnati, OH, 2005.



Nien-Hwa Linda Wang

PhD., Minnesota, 1978

Professor

Research Areas

Chemical and Biochemical Separations, Ion Exchange, Adsorption, Simulated Moving Bed Chromatography, Complex Adaptive Systems

Selected Professional Activities

Fellow, American Institute for Medical and Biological Engineering

Director of the International Adsorption Society (May 2001-May 2007)

Selected Invited lectures

"Size-Exclusion Simulated Moving Bed for Insulin Purification," Asia-Pacific Biochemical Engineering Conference 2005, Jeju Island, Korea, May, 2005.

Selected Publications

Lee, K. B., C. Chin, Y. Xie, G. Cox, and N.-H. L. Wang, "Standing Wave Design of a Simulated Moving Bed under a Pressure Limit for Enantioseparation of Phenylpropanolamine," *IEC Research*, 44(9), 3249-3267 (2005).

Xie, Y.; D. Phelps; C.H. Lee, M. Sedlak; N. Ho.; and N.-H.L. Wang, "Comparison of Two Adsorbents for Sugars Recovery from Biomass Hydrolysate," *IEC Research*, in press.

Xie, Y., C. Chin, D. Phelps, C. H. Lee, K.B. Lee, S. Y. Mun, and N.-H. L. Wang, "A Five-Zone Simulated Moving Bed for Isolation of Six Sugars from Biomass Hydrolyzate," *IEC Research*, 44, 0004-9920 (2005).

Lee, K.B., S. Y. Mun, F. Cauley, G. Cox, and N.-H. L. Wang, "Optimal Standing Wave Design of Nonlinear Simulated Moving Bed Systems for Enantioseparation," *IEC Research*, in press.

Mun, S.Y., C. Chin, Y. Xie, and N.-H. L. Wang, "Standing Wave Design of Carousel Ion Exchange Process for the Removal of Zinc Ions from a Protein Mixture," *IEC Research*, in press.

Mun, S. Y. & N.-H. L. Wang, "Insulin Wave Dynamics in Size-Exclusion Simulated Moving Bed with Residence Time Control," *IEC Research*, in press.

Selected Conference Presentations

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11: SMB Technology, Y. Xie, C. Chin, D. S. C. Phelps, C.-H. Lee, K.-B. Lee, S. Y. Mun, and N.-H. L. Wang, "A Five-Zone Simulated Moving Bed for Isolation of Six Sugars from Biomass Hydrolyzate."

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11: Fundamentals of Adsorption and Ion Exchange II, C. M. Yu, S. Mun, N.-H. L. Wang, "Effects of Reversible Association on Size Exclusion Chromatography of Proteins."

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11: Adsorption from Mixtures, S. Mun, C. Chin, Y. Xie, and N.-H. L. Wang, Standing Wave of Carousel Ion Exchange Processes for the Removal of Zinc Ions from a Protein Mixture."

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11, Poster: Adsorption and Ion Exchange, H.-J. Lee, C. Chin, and N.-H. L. Wang, "The Role of Dissociation Reaction on Simulated Moving Bed Purification of Lactic Acid."

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11: Liquid Phase Adsorption, K.-B. Lee, G. B. Cox, and N.-H. L. Wang, "Effects of System Parameters and Material Properties on Productivity and Desorbent Consumption in Chiral SMB Separation."

2005 AIChE Annual Meeting, Cincinnati, OH, Nov. 7-11: Protein Chromatography and Chiral Resolution of Biomolecules, R. Kasat, K. Thomson, H. Hillhouse, N.-H. L. Wang, and E. I. Franses, "Molecular Mechanisms of Selective Sorption of Chiral Enantiomer on Amylose-Based Sorbents."



Phillip C. Wankat

Ph.D Princeton University, 1970

*C. L. Lovell Distinguished Professor
Director, Undergraduate Degree Programs,
Department of Engineering Education*

*Shreve Prize in Chemical Engineering, 2005
Engineering Mentoring Award, Purdue, 2005*

Research Areas

Adsorption Operations, Large-scale Chromatography, Distillation, Engineering Education

Selected Invited lectures

“Survey of K-12 Engineering-Oriented Student Competitions,” Invited paper ASEE/AaeE Global Colloquium on Engineering Education, Sydney, Australia, September 2005.

“Effective, Efficient Teaching,” Inaugural Seminar in Teaching and Learning Seminar Series, Monash University, Clayton (Melbourne) Australia, September 21, 2005.

“Improving Teaching has Failed – We Need Better Learners and More Effective Teaching,” University of Queensland, Brisbane, Australia, September 23, 2005.

“Effective, Efficient Teaching,” University of Canterbury, Christchurch, New Zealand, October 3, 2005.

“Effective, Efficient Teaching,” and “Interdisciplinary Engineering (IDE): A Flexible Degree Program for Students Who Don’t Fit in Standard Programs,” Waikato University, Hamilton, New Zealand, October 4, 2005.

“Teaching with Computer Simulations,” University of Auckland, Auckland, New Zealand, October 5, 2005.

Selected Publications

Wankat, P. C., *Separation Process Engineering*, Prentice-Hall, Upper Saddle River, NJ, 2007. 738 pages plus separate Solution Manual. [Second edition of *Equilibrium-Staged Separations*].

Brannan, K. P. and P. C. Wankat, “Survey of First-Year Programs,” Proceedings ASEE 2005 Annual Conference, CD, session 1353. Available from the ASEE web site at http://asee.org/acPapers/2005-236_Final.pdf.

Hur, J.-S. and P. C. Wankat, “Two-Zone SMB Chromatography for Center-Cut Separations,” *Ind. Engr Chem. Research*, 45, 1426-1433, (2006).

Jin, W. and P. C. Wankat, “Scaling Rules and Increasing Feed Rates in Two-Zone and Four-Zone SMB Systems,” *Ind. Engr Chem. Research*, 45, 2793-2807 (2006).

Abunasser, N. and P. C. Wankat, “Improving the Performance of One Column Analogs to SMBs,” *AIChE Journal*, 52, 2461 (2006).

Wankat, P. C., and F. S. Oreovicz, “Teaching Prospective Engineering Faculty How to Teach,” *Intl. J. Engr. Educ.*, 21 (5) 925-930 (2005).

Selected Conference Presentations

Brannan, K. P. and P. C. Wankat, “Survey of First-Year Programs,” ASEE 2005 Annual Conference, Portland, OR, June 2005, session 1353. Winner of ASEE Freshman Program Division Best Paper Award, the Professional Interest Council III (PIC III) Best Paper Award and the Best Conference Paper Award. Published in CD of Proceedings ASEE 2005 Annual Conference.

Wankat, P. C., “Learning from the Enemy: Educational Methods of Private, For-Profit Colleges,” ASEE 2006 Annual Conference, Chicago, IL, June 2006. Published in CD of Proceedings ASEE 2006 Annual Conference, June 2006.

Hur, J.-S. and P. C. Wankat, “Simulated Moving Bed Systems for Center-Cut Separation from Quaternary Mixtures,” AIChE Annual Meeting, Cincinnati, Ohio, November 2005.

Jin, W. and P. C. Wankat, “Parallel Two-Zone and Four-Zone Hybrid SMB Systems for the Separation of p-xylene,” AIChE Annual Meeting, Cincinnati, Ohio, November 2005.



You-Yeon Won

PhD, Minnesota, 2000

*Assistant Professor
Assistant Professor of Materials Science Engineering
(by courtesy)*

Research Areas

Polymers and complex fluids, Nanobioengineering

Selected Professional Activities

Vice-Chair, Thermodynamics at Nanoscale session at 2005 AIChE Annual Meeting in Cincinnati, OH.

Selected Invited lectures

“Virus-Mimetic DNA Encapsulation Using Novel Triptych Polymers” Low-Energy Neutron Scattering (LENS) Seminar, Indiana University Cyclotron Facility (IUCF), Bloomington, IN, November 15, 2005.

Selected Publications

“Nonionic Block Copolymer Wormlike Micelles,” Y.-Y. Won, F. S. Bates, in *Giant Micelles: Properties and Applications* (Editors: R. Zana, E. W. Kaler), CRC Press/Taylor & Francis, Boca Raton, FL, 2006.

“Self-Consistent Field (SCF) Analysis of Mixed Polyelectrolyte and Neutral Polymer Brushes,” K. N. Witte, Y.-Y. Won, *Macromolecules*, in press, 2006.

“Inhibitive Chain Transfer to Ligand in the ATRP of n-Butyl Acrylate,” R. Sharma, A. Goyal, J. M. Caruthers, Y.-Y. Won, *Macromolecules*, 39(14), 4680-4689, 2006.

“Effect of Temperature on Carbon Black Agglomeration in Hydrocarbon Liquid with Adsorbed Dispersant,” Y.-Y. Won, S. P. Meeker, V. Trappe, D. A. Weitz, N. Z. Diggs, J. I. Emert, *Langmuir* 21(4), 924-932, 2005.

“Rubbery Graft Copolymer Electrolytes for Solid-State, Thin-Film Lithium Batteries,” P. E. Trapa, Y.-Y. Won, S. C. Mui, E. A. Olivetti, B. Huang, D. R. Sadoway, A. M. Mayes, S. Dallek, *Journal of the Electrochemical Society* 152(1), A1-A5, 2005.

Selected Conference Presentations

“Virus-Mimetic DNA Encapsulation Using Novel Polyelectrolyte Triblock Copolymers,” Y.-Y. Won, R. Sharma, MRS Spring Meeting, San Francisco, CA, April 2006.

“Virus-Mimetic DNA Encapsulation Using Novel ABC Triblock Copolymers,” R. Sharma, Y.-Y. Won, APS March Meeting, Baltimore, MD, March 2006 (This presentation was mentioned in the APS Meeting News Release in March 2006).

“Conformational Properties and Phase Behavior of Mixed Brushes between Charged and Neutral Polymers: SCF Modeling Using the Edwards Hamiltonian Approach,” K. Witte, Y.-Y. Won, APS March Meeting, Baltimore, MD, March 2006.

“Calcium Alginate Gel Beads Synthesis by Electrodispersion in Vegetable Oils,” Y. Zhao, Y.-Y. Won, M. T. Harris, AIChE Annual Meeting, Cincinnati, OH, October/November 2005.

“Novel Triptych Polymers for Virus-Mimetic DNA Encapsulation,” R. Sharma, Y.-Y. Won, AIChE Annual Meeting, Cincinnati, OH, October/November 2005.

“Synthesizing Model Block Copolymers via ATRP: The Utility of Kinetic Modeling in Guiding Experiments,” R. Sharma, Y.-Y. Won, AIChE Annual Meeting, Cincinnati, OH, October/November 2005.