1998-1999 The School of

Chemical Engineering

Faculty Summary

Lyle F. Albright

**1955*

Professor Emeritus

Degrees

BS, University of Michigan, 1943

MS, University of Michigan, 1944

PhD, University of Michigan, 1950

Interests

Kinetics and processes of organic reactions (especially pyrolysis, alkylation of isobutane, nitration, and hydrogenation of vegetable oils)

High polymers and polymerization

Gasification and liquefaction of coal

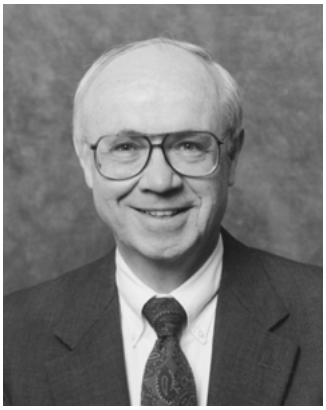
Pulping of wood chips for paper production

** Year of joining the faculty.*

Ronald P. Andres

1981

Engineering Research Professor



Degrees

BS, Northwestern University, 1959

PhD, Princeton University, 1962

Interests

Ultrafine particles

Nanostructured materials

Nanoelectronic devices

Catalysis

Scanning Probe Microscopy

Research Areas

Molecular Electronics: The field of "molecular electronics" is in its infancy and demonstrations of sophisticated electronic functions by molecular based systems have been limited. However, an interdisciplinary team of researchers at Purdue has shown that metal nanocrystals can be "wired" to each other by means of conjugated organic molecules having appropriate end groups and these supramolecular systems show great promise in a wide range of ultra-high-density electronic and information storage applications. We are currently exploring applications of this technology in the fabrication of nanoelectronic devices and chemical sensors. Our ability to deposit uniform monolayers of chemically linked metal clusters is also an exciting enabling technology for semiconductor electronics. Among the potential applications that are being studied are: nanometer resolution etch masks, low resistance nanocontacts, and interconnect lines that are self-aligning, self-healing and conformal.

Synthesis of Ultrafine Metal Particles: Ultrafine metal particles or clusters with diameters in the nanometer size range have unique size-dependent electronic and physical properties. Nanostructured materials such as solids produced by consolidation of nanoscale powders or catalysts produced by dispersing nanoscale metal clusters on nonreactive supports also exhibit unique properties. The key to taking advantage of these enhanced properties is a technique for synthesizing the ultrafine particles of interest at high production rates and low cost. We have developed several aerosol based methods for nanoparticle synthesis and are involved in extending our understanding of these processes by theoretical modeling and experimental scale up.

Self-Assembly of 2-D and 3-D Nanoparticle Structures: Many of the most exciting materials applications of ultrasmall clusters require that

these particles be assembled into regular 2-D or 3-D superlattices. The only feasible way to accomplish this task appears to be via self-assembly, which can be defined as a process in which a supramolecular hierarchical organization is spontaneously established in a complex system of interlocking components. We have developed methods for the engineered self-assembly of cluster superlattices and are involved in improving these techniques and extending our understanding of the basic physics of the the self-assembly process. The self-part of self-assembly refers to the fact that the process is driven by an overall free energy drop between the unassembled units and the final assembly. Thus, understanding the thermodynamics of nanoparticle systems is crucial. The speed and the scale-up of the self-assembly process are also important considerations.

Scanning Probe Microscopy: The Atomic Force Microscope (AFM) uses a sharp probe attached to a flexible cantilever to profile the morphology of a sample surface. Although a powerful technique for determining nanoscale structure, because of the finite size of the probe tip, an AFM has limited lateral resolution and tends to deform "soft" samples. We have largely overcome these problems by using a carbon nanotube as the probe and by depositing a metal cluster of controlled size at the tip of the nanotube to serve as the effective probe tip. With this new probe we are able to resolve for the first time the nanoscale structure of "soft" surfaces. This capability opens up the possibility of using an AFM to image a wide range of biochemical and biomedical nanostructures.

Publications

R.P. Andres, S. Datta, D.B. Janes, C.P. Kubiak, R. Reifenberger, "The Design, Fabrication and Electronic Properties of Self-Assembled Molecular Nanostructures," *Handbook of Nanostructured Materials and Nanotechnology* (ed. H.S. Nolwa) Academic Press (1999).

D. Lovall, M. Buss, R.P. Andres, R. Reifenberger, "Resolving the Atomic Structure of Supported Nanometer-size Au Clusters," *Phys. Rev. B, 58,* 15889 (1998).

S. Datta, D.B. Janes, R.P. Andres, C.P. Kubiak, R.G. Reifenberger, "Molecular Ribbons," *Semicond. Sci. Technol., 13*, 1347 (1998).

Meeting Presentations

"Advances in Scanning Force Microscopy," Midwest Microscopy and Microanalysis Society, Purdue University, West Lafayette, IN, October 1998.

"The Nano-Nose: a Cluster-Based, Multi-Spectral, Chemical Sensor," NSF Workshop: Vision for Nanotechnology R&D in the Next Decade, Washington, DC, January 1999.

Invited Lectures

"Self-Assembly of a Patterned 2D Network of Metal Clusters Joined by Conjugated Organic Molecules," American Chemical Society, Boston, MA, August 1998.

"Aerosol Synthesis of Functional Nanomaterials," First Joint ESF-NSF Symposium on Aerosols for Nanostructured Materials and Devices, Edinburgh, Scotland, September 1998.

"Aerosol Synthesis of Functional Nanostructures," Chemical Engineering Department, Texas A&M University, College Station, TX, October 1998.

"Aerosol Synthesis of Functional Nanostructures" and "Electronic Behavior of Metal Quantum Dots Interconnected by Conjugated Organic Molecules," Chemical Engineering Department and Center for Nanotechnology, University of Washington, Seattle, WA, October 1998.

"A Linked Cluster Network Based Chemical Sensor: A Nano-Nose," Nanotechnology and Sensor Workshop, Purdue University, April 1999.

"Aerosol Synthesis of Metal Nanocrystals and Their Self-Assembly into Electronic Nanostructures," Department of Electrical and Computer Engineering and Computer Science, University of Cincinnati, May 1999.

Osman Basaran

1995

Professor

Degrees

BS, Massachusetts Institute of Technology, 1978

Ph D, University of Minnesota, 1984

Interests

Computational fluid dynamics (CFD) and finite element analysis

Nonlinear dynamics in ordinary and micro gravity

Dynamics of complex fluids

Experimental fluid dynamics: ultra high-speed visualization and digital imaging

Interfacial phenomena; surface and bulk rheology

Ink-jet printing and atomization coating

Biochips, MEMS, miniaturization, and massively parallel DNA analysis and drug discovery

Electric field-enhanced separations

Drop breakup in laminar and turbulent flows

Awards and Major Appointments

Member, AIChE National Fluid Mechanics Programming Committee (1992-present)

Member, AIChE Coating Symposium Steering Committee (1996-present)

Research Areas

The research program is motivated by practical applications ranging from ink-jet printing to minituarization of bioanalytical instrumentation to separations. In particular, the group is involved in developing the scientific underpinnings of applications including but not limited to so-called discontinuous coating flows such as ink-jet printing, atomization coating, spray painting, and crop spraying o electrically-enhanced separations measurement of interfacial and bulk rheological properties micro fluid dynamics of flows arising in biochip processors and devices for carrying out “chemistry on a chip.” Making progress in these areas requires investigation and solution of several key thorny issues at the forefront of physical science such has how liquids break and coalesce and how liquids slip on solid surfaces, among others. In ink-jet printing, atomization coating and painting, and crop spraying, two central problems are the generation of drops from a nozzle and the deposition of drops that are thereby generated on a suitable substrate. Both of these

problems are under study using computational and experimental techniques. Of particular interest to the group in these studies are the effects of surfactants and dynamic surface tension (DST), non-Newtonian rheology and shear-thinning behavior of liquids, and viscoelasticity and extensional viscosity of liquids. The group has pioneered and continues to develop novel finite element algorithms for calculating the large-amplitude deformation and breakup of liquid drops. An area of current emphasis is modeling of ejection of tens of drops in a sequence from capillary tubes and other nozzles to study occurrence of period doubling bifurcations and of routes to chaos. On the experimental side, the group leads the pack in direct visualization of drop dynamics events with an astounding digital image recording rate of one hundred million frames per second. The group has recently pioneered novel techniques for dispensing high-viscosity drops from drop-on-demand ink-jet printers. In separations, the use of electric fields in enhancing the efficiency of separations such as solvent extraction is under scrutiny. Here interest is focused on how electric fields can be used to produce mono-sized drops and eliminate satellite droplets. Progress in this effort is being expedited by the development of novel algorithms to predict drop formation phenomena in the presence of an external electric field. Efforts are also under way to use a two-component Phase Doppler Anemometer that is capable of measuring the size and two components of the velocity of drops in an electrospray. In parallel to PDA, high-speed visualization at 12,000 frames / sec and ultra high-speed visualization at 100,000,000 / sec are being utilized to gain insights into drop formation phenomena. Novel equipment has either been built recently or is in the process of construction to measure dynamic surface tension and extensional viscosity. The Purdue growing drop apparatus for measuring DST can probe surface tension variations on time scales as short as 1 / 12th of a millisecond. The new Purdue extensional rheometer is under development. These novel pieces of equipment allow the scientist / engineer to measure surface and bulk properties on time scales and dilatation / extension rates of relevance to industrial practice. There is great interest in minituarizing devices used for bioanalysis and coming up with efficient and accurate techniques for DNA analysis and sequencing. Equally important is development of techniques that can be used in rapid screening of new drugs. A common thread in these lifescience applications is the manipulation of ultra-small volumes of liquids, such as in dispensing microdoses of solutions of oligonucleotides onto surface-treated substrates or in pumping blood or reagents through micron-size channels Several such problems are being studied in collaboration with various industrial companies.

Publications

Ambravaneswaran, B. and Basaran, O.A. 1999 Effects of insoluble surfactants on the nonlinear deformation and breakup of stretching liquid bridges. Phys. Fluids 11, 997-1015.

Notz, P.K. and Basaran, O.A. 1999 Dynamics of drop formation in an electric field. J. Colloid Interface Sci. 213, 218-237.

Notz, P. K. and Basaran, O. A. 1998 Dynamics of Drop Formation in an Electric Field. Proceedings of ILASS-Americas 1998, 180-184.

Wilkes, E. D. and Basaran, O. A. 1998 Dynamics of Drop Formation at Finite Reynolds Numbers. Proceedings of ILASS-Americas 1998, 391-

395.Basaran, O.A., “Dynamics of Drop Formation,” Chemical Engineering Department and the Levich Institute, City College of CUNY, New York, New York, May 4, 1999.

Invited Lectures

Basaran, O. A., “Effects of Electric Fields on the Dynamics of Drop Formation from a Nozzle,” IBC’s 3rd Annual Microfabrication and Microfluidic Technologies Conference, San Francisco, California, August 6-7, 1998. [Invited plenary lecture]

Basaran, O. A., “Role of Surface and Bulk Rheology in Dynamics of Drop Formation and Impact,” IBC’s International Conference on Massively Parallel DNA Analysis, San Francisco, California, August 10-11, 1998. [Invited plenary lecture]

Basaran, O. A., “Drop Formation at Finite Reynolds Numbers: Interface Overturning, Effects of Electric Fields, and More,” IUTAM Symposium on Nonlinear Wave Behavior in Multi-Phase Flow, University of Notre Dame, Indiana, July 7-9, 1999. [Invited lecture] Ambravaneswaran, B. and Basaran, O.A., “Effects of Insoluble Surfactants on the Nonlinear Deformation and Breakup of Stretching Liquid Bridges,” 9th International Coating Science and Technology Symposium, 17-20 May, 1998, University Delaware, Newark, Delaware.

Meeting Presentations

Kim, J. S. and Basaran, O.A., “Effect of a Tangential Electric Field on the Deformation and Breakup of a Stretching Bridge of a Perfectly Insulating Liquid,” 9th International Coating Science and Technology Symposium, 17-20 May, 1998, University Delaware, Newark, Delaware.

Yildirim, O. E. and Basaran, O.A., “ Deformation and Breakup of Non-Newtonian Liquid Bridges Undergoing Uniaxial Extension,” 9th International Coating Science and Technology Symposium, 17-20 May, 1998, University Delaware, Newark, Delaware.

Notz, P. K. and Basaran, O.A. (speaker), “Drop Formation in an Electric Field: Drop Size Control and Elimination of Satellites in Discontinuous Coating Flows,” 9th International Coating Science and Technology Symposium, 17-20 May, 1998, University Delaware, Newark, Delaware.

Wilkes, E. D. and Basaran, O.A. (speaker), “Dynamics of Formation of Single Drops in a Prototypical Discontinuous Coating Flow,” 9th International Coating Science and Technology Symposium, 17-20 May, 1998, University Delaware, Newark, Delaware.

Whitaker, J., Ambravaneswaran, B. and Basaran, O.A., “Effects of Insoluble Surfactants on the Nonlinear Dynamics of Oscillating Liquid Bridges,” 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Panditaratne, J., Ambravaneswaran, B. and Basaran, O.A., “Effects of Contact Line Radius and Contact Line Motion on the Deformation and Breakup of Stretching Liquid Bridges,” 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Ambravaneswaran, B. and Basaran, O.A., “Comparison of predictions of one- and two-dimensional models of drop formation,” 51st Annual

Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Notz, P.K. and Basaran, O.A., "Dynamics of Formation of Dielectric Drops from a Capillary in an Electric Field," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Basaran, O.A. and Basaran, O.A., "Drop Formation from a Capillary with an Oscillatory Flow Rate," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Wilkes, E.D. and Basaran, O.A., "Drop Ejection from an Oscillating Rod," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Chen, A. U. and Basaran, O.A., "Effects of a Radial Electric Field on the Nonlinear Deformation and Breakup of a Stretching Bridge of a Conducting Liquid," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Phillips, S., Wilkes, E.D. and Basaran, O.A., "Transitions in the Dynamics of Drop Formation from a Capillary with Increasing Flow Rate," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Yildirim, O.E. and Basaran, O.A., "Formation of Drops of non-Newtonian Liquids from a Capillary," 51st Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 22-24 November 1998, Philadelphia, Pennsylvania.

Ambravaneswaran, B., McGough, P., Whitaker, J. and Basaran, O.A., " Effects of Insoluble Surfactants on the Nonlinear Deformation of Oscillating Liquid Bridges," AIChE 1998 Annual Meeting, 15-20 November 1998, Miami Beach, Florida.

Notz, P.K. and Basaran, O.A., "Effects of Physical Properties on the Dynamics of Drop Formation from a Capillary in an Electric Field," AIChE 1998 Annual Meeting, 15-20 November 1998, Miami Beach, Florida.

Wilkes, E.D. and Basaran, O.A., " Dynamics of Drop Formation from Capillaries under Steady and Oscillatory Flow Conditions," AIChE 1998 Annual Meeting, 15-20 November 1998, Miami Beach, Florida.

Chaired Conferences/ Symposia

Session Chair, "Coating Process Technology, 9th International Coating Science and Technology Symposium, 17-20 May 1998, University of Delaware, Newark, Delaware.

Facilitator, Panel Discussion on "Deposition and Coatings," 11th Annual Conference on Liquid Atomization and Spray Systems (ILASS), Sacramento, California, May 1998.

Gary E. Blau

1998

Visiting Industrial Professor

Degrees

BASc, University of Waterloo, 1964

MSc, Stanford University, 1966

PhD, Stanford University, 1968

Interests

Mathematical Model Building of Engineering Systems

Operations Research

Optimization

Applied Statistics

Environmental Systems

Uncertainty / Risk Analysis

Research Areas

The chemical process industries and pharmaceutical industries are faced with the challenge of demonstrating increased productivity with leaner organizations in a highly competitive global economy. Dr. Blau's research focuses on the development and application of decision-making tools which exploit recent developments in computer and information technologies to help both managers and engineers successfully manage risk in this environment. Specifically, he is addressing the many issues associated with the development of new products and processes. This includes the treatment of uncertainty during all aspects of the product life cycle from ideation / discovery through product commercialization. Particular emphasis is on recent developments in decision analysis, forecasting, discrete even simulation, risk analysis and probabilistic optimization.

Publications

Third International Conference on Foundations of Computer-Aided Process Operations, Edited by Joseph F. Pekny & Gary E. Blau, AICHE Symposium Series, Volume 94, 1998

Schmidt, C.W., I. Grossmann, G. E. Blau, "Optimization of Industrial Scale Scheduling Problems in New Product Development," Proceedings of ESCAPE 9, Brugge, Belgium, 1998.

G.E. Blau and Kuenker, K.E., "Culture Shift: Positioning Technical Computing to Enable Sustained Profitability in the Specialties Business," Proceedings of Foundations of Computer Aided Operations Conference, Snowbird, UT, 1998.

Schnelle, K., D. Campbell, G.E. Blau, "Bringing New Specialty Chemicals to Market - A Nightmare in Planning and Scheduling," Proceedings of Foundations of Computer Aided Operations Conference, Snowbird, UT, 1998.

Invited Lectures

"Resource Management in New Product Developement Programs," Alza Corporation, Mountain View, California, 1999.

"Project Selection and Risk Management in New Product Development Pipelines," Air Products & Chemical Inc., Allentown, Penna, 1999.

Steele, K. and G.E. Blau, "The Terrible / Wonderful Problem of Product Planning and Prioritization in the Agrochemicals Business," Gordon Research Conference on Statistics in Chemistry and Chemical Engineering, NH, 1998.

Short Courses

"Process Optimization through Experimental Design": Two-day short course for industrial scientists and Managers, 1999

James M. Caruthers

1977

Professor

Degrees

SB (Chem), Massachusetts Institute of Technology, 1975

SM, Chemical Engineering, Massachusetts Institute of Technology, 1975

PhD, Chemical Engineering, Massachusetts Institute of Technology, 1977

Interests

Nonlinear viscoelasticity of polymer solids

Structure-property relationships in polymers

Chemical and physical aging of polymers and polymer composites

Solid state NMR of chemical reactions in solid polymers

Application of AI methods for design of materials

Awards and Major Appointments

Co-Director of Center for Materials Design, Purdue University, 1999-present

National Research Council: Standing Committee on the Program and Technical Review of the U.S. Army Chemical and Biological Defense Command, 1995-1998

Research Areas

Prof. Caruthers' research is focused on how changes in molecular architecture control the engineering properties of high performance polymers, polymer composites, and other engineering materials. The research is a blend of experiments, the development of physically motivated theoretical models, and implementation of the models in extremely large computer codes in order to solve real manufacturing and design problems.

Prof. Caruthers and his group have investigated the mechanical, thermal, and rheological behavior of amorphous polymers that are used in a variety of high performance aerospace, automotive, and electronic applications. Polymers are processed as a fluid, solidified by cooling, and then used as an engineering material in the solid state. The flow process and solidification history can significantly alter the engineering properties of the resulting solid. however, most existing models do not incorporate the effects of the deformation / thermal history encounter during processing in a reasonable manner. A new nonlinear viscoelastic constitutive equation has been developed that naturally includes the nonlinear rheological behavior in the melt, the complex vitrification processes in the glass transition region, and the 3D-nonlinear deformation behavior in the resulting solid. In order to validate the model an

extensive set of experimental data are being generated at Purdue, Sandia National Laboratory, and at several industrial laboratories - data which when complete will be most extensive collection of experimental results for an engineering polymer. Finally, Prof. Caruthers' group is collaborating with computational mechanics group at Sandia to incorporate the constitutive model into extremely large finite element code in order to solve real world manufacturing and design problems.

A second research area is concerned with the effects of chemical reaction on the mechanical behavior of engineering polymers. Polymer is currently being used in a number of high performance applications, where they may be exposed to thermal and chemical environments that cause degradation. Since the service lifetime of a component maybe as long as 30 years, it is obviously impossible to just experimentally measure the effect of chemical degradation. ^{1}H, ^{13}C, and ^{15}N solid state NMR have been used to directly measure the degradation mechanisms in several polyimide polymers that are used in high temperature applications. In particular the ^{15}N NMR studies have clearly identified the chemical degradation pathways and kinetics for the polyimide materials. The group is currently working how to incorporate mechanistically sound kinetic models for the cure reaction, hydrolytic degradation, and thermoxidative degradation into a nonlinear constitutive equation so that the lifecycle performance of these important engineering materials can be rationally predicted.

A third research area is collaboration with Prof. Venkatasubramanian in the application of Artificial Intelligence methods for the design of complex mixture such as filled polymers, gas/oil additive, etc. We are currently working with a number of significant industrial sponsors on real industrial product design problems. Our group has developed hybrid neural network (NN) models that incorporate fundamental knowledge when available, empirical rules from expert human material formulators, and statistical models from experimental data. A second activity is concerned with the development of Genetic Algorithms (GA) for the determination of the necessary chemical structure and mixture composition to meet the material design requirement for a specific engineering application. The NN and GA models are being developed in collaboration with several major materials companies in order to develop of new materials for existing and future engineering applications. This research activity has recently received considerable national attention being recognized in 1998 as one of the top 50 R&D technologies in all fields of science and engineering and including both academic and industrial research groups. Because of the success of this novel technology, we have recently established the Center for Materials Design to partner with a variety of industrial sponsors in well-defined application areas.

Publications

C.R. Novenario, J.M. Caruthers, and K.C. Chao, "Heat Capacity of Polymer Melts from the Polymer Chain-of-Rotators Equation of State," *Journal Applied Polymer Sci, 67,* 841, 1998.

D.B. Curliss, B.A. Cowans, and J.M. Caruthers, "Cure Reaction Pathways of Bismaleimide Polymers: A Solid State ^{15}N NMR Investigation," *Macromolecules, 31*, 6776, 1998.

C.R. Novenario, J.M. Caruthers, and K.C. Chao, "Chain-of-Rotators Equation of State for Polar and Non-polar Substances and Mixtures," *Fluid Phase Equilibria, 142*, 83, 1998.

C.R. Novenario, J.M. Caruthers, and K.C. Chao, "Vapor-Liquid Equilibrium of Polymer + Solvent Mixtures by the Chain-of-Rotators Equation of State," *Industrial & Engineering and Chemistry Research, 37*, 3142, 1998.

J.M. Caruthers, D.B. Adolf, and R.S. Chambers, "A Nonlinear Viscoelastic Constitutive Model for Engineering Polymers: 1. Constitutive Development," Proceedings of the SEM Annual Conference on Theoretical, Experimental and Computational Mechanics, Society of Experimental Mechanics, p. 866, 1999.

R.S. Chambers, D.B. Adolf, and J.M. Caruthers, "A Nonlinear Viscoelastic Constitutive Model for Engineering Polymers: 2. Experimentation and Computing," Proceedings of the SEM Annual Conference on Theoretical, Experimental and Computational Mechanics, Society of Experimental Mechanics, p. 175, 1999.

P. Ghosh, S. Katare, P. Patkar and J. M. Caruthers, "A Kinetic Model for Accelerated Sulfur Vulcanization for Natural Rubber," ACS-Rubber Division, Paper No. 7, Orlando, FL (1999).

P. Ghosh and J. M. Caruthers, "Constitutive Model for Predicting Stress Response of Sulfur Vulcanized Rubbers During Simultaneous Deformation and Chemical Aging," ACS-Rubber Division, Paper No. 7, Orlando, FL (1999).

Invited Lectures

"A Model for Nonlinear Viscoelasticity of Polymer Glasses," Kodak Corp, Rochester, NY, July, 1998.

"Application of AI Techniques for the Design of Filled Polymers," Caterpillar Corp., Peoria, IL, August, 1998.

"A Rational Methodology for Predicting Lifetime Performance of Engineering Polymers in Degradative Environments," 2nd International Conference on Elastomer Service Life Prediction, Akron, OH, September, 1998. Keynote address.

"Nonlinear Viscoelastic Constitutive Models for Predicting the Lifetime Performance of Polymer Matrix Composites," Air Force Resarch Laboratory, Wright Patterson AFB, Dayton, OH, September, 1998.

"Constitutive Models for Amorphous Polymers that Incorporate Cure and Degradative Chemical Aging." Lawrence Livermore National Laboratory, Livermore, CA, January, 1999.

Meeting Presentations

"A Complete Second Order Nonlinear Viscoelastic Model for Amorphous Polymers," G. Medvedev, P. Shirkhande and J.M. Caruthers, Society of Rheology, Monterey, CA, October 1998.

"Comparison of the Volume and Temperature Dependence of Various Log(a) Shift Models with Experimental Data," S.J. Lee , G. Medvedev and J.M. Caruthers, Society of Rheology, Monterey, CA, October 1998.

"The Effect of Composition Fluctuations on the Network Structure and Cure Kinetics of Network Polymers, "R. Sy-Siong-Kiao and J.M. Caruthers, AIChE Annual Meeting, Miami, FL, Nov. 1998.

"Constitutive Model for Pressure-Volume-Temperature Behavior of Polymeric Glasses: The Effect of Density Fluctuations," G. Medvedev, S.J. Lee and J.M. Caruthers, AIChE Annual Meeting, Miami, FL, Nov. 1998.

"Effect of compositional fluctuations on the cure kinetics of network-polymers," R. Sy-Siong-Kiao and J.M. Caruthers, APS Meeting, Atlanta, GA, March, 1999. (poster)

"Effect of Network Structure on the Glass Transition Temperature in Amine Cured Epoxies," R. Sy-Siong-Kiao and J.M. Caruthers, APS Meeting, Atlanta, GA, March, 1999.

"Analysis of Physical Aging of Amorphous Copolyester using the GKAC Model," J.M. O'Reilly, J.M. Caruthers and P. Shrikhande, APS Meeting, Atlanta, GA, March, 1999.

"Modeling of the Physical Aging behavior of Polycarbonate," P. Shrikhande, J.M. Caruthers and J.M. O'Reilly, APS Meeting, Atlanta, GA, March, 1999.

"Mesoscopic model of structural relaxation in glass," G.A. Medvedev, S.-J. Lee and J.M. Caruthers, APS Meeting, Atlanta, GA, March, 1999.

"A Nonlinear Viscoelastic Constitutive Model for Engineering Polymers: 1. Constitutive Development," J.M. Caruthers, D.B. Adolf, and R.S. Chambers, Society of Experimental Mechanics Annual Meeting, Cincinnati, OH, June, 1999.

"A Nonlinear Viscoelastic Constitutive Model for Engineering Polymers: 2. Experimentation and Computing," R.S. Chambers, D.B. Adolf, and J.M. Caruthers, Society of Experimental Mechanics Annual Meeting, Cincinnati, OH, June, 1999.

"Quantitative Model for the Cure Kinetics of Sulfur Vulcanization of Natural Rubber," P. Gosh, P. Patkar, S. Katare and J.M. Caruthers, ACS Rubber Division Annual Meeting, Orlando, FL, Sept. 1999

"Constitutive Model for Predicting the Stress Response of Sulfur Vulcanized Rubbers During Long Term Chemical Aging," P. Gosh, S. Katare and J.M. Caruthers, " ACS Rubber Division Annual Meeting, Orlando, FL, Sept. 1999.

"The Relationship Between the Energy Landscape and Viscoselastic Relaxation for Glassy Materials," R. Bhatia, G. Medvedev, D. Corti, and J.M. Caruthers, Society of Rheology, Madison, WI, Oct. 1999.

"Critical Evaluation of a Nonlinear Viscoelastic Constitutive Model for Glassy Polymers," J.M. Caruthers, D.B. Adolf, R.S. Chambers, G. Medvedev, and P. Shrikhande, Society of Rheology, Madison, WI, Oct. 1999.

"Constitutive Model for Predicting the Stress Response of Sulfur Vulcanized Rubbers During Simultaneous Deformation and Chemical Aging," P. Gosh, S. Katare and J.M. Caruthers, Society of Rheology, Madison, WI, Oct. 1999.

"Meso-scale Model Including Fluctuations to Describe Volume Relaxation in Polymeric Glasses," G. Medvedev and J.M. Caruthers, Society of Rheology, Madison, WI, Oct. 1999.

"The Relationship Between the Energy Landscape and Viscoselastic Relaxation for Glassy Materials," R. Bhatia, G. Medvedev, D. Corti, and J.M. Caruthers, AIChE Annual Meeting, Dallas, TX, Nov. 1999.

"Critical Evaluation of a Nonlinear Viscoelastic Constitutive Model for Glassy Polymers," J.M. Caruthers, D.B. Adolf, R.S. Chambers, G. Medvedev, and P. Shrikhande, AIChE Annual Meeting, Dallas, TX, Nov. 1999.

"Constitutive Model for Predicting the Stress Response of Sulfur Vulcanized Rubbers During Simultaneous Deformation and Chemical Aging," P. Gosh, S. Katare and J.M. Caruthers, AIChE Annual Meeting, Dallas, TX, Nov. 1999.

"Meso-scale Model Including Fluctuations to Describe Volume Relaxation in Polymeric Glasses," G. Medvedev and J.M. Caruthers, AIChE Annual Meeting, Dallas, TX, Nov. 1999.

"The Cure Kinetics of Amine-Epoxy Thermosets and the Evolution of Engineering Properties," R. Sy-Siong-Kiao and J.M. Caruthers, AIChE Annual Meeting, Dallas, TX, Nov. 1999.

David S. Corti

1998

Assistant Professor

Interests

Statistical Thermodynamics

Metastable Liquids

Nucleation Phenomena

Colloidal Dispersions

Molecular Simulation Techniques

Research Areas

Entropic Control of Colloidal Stability, Phase Transition, and Particle Deposition

The ability to predict the behavior of colloidal dispersions rests upon our knowledge of the forces that arise between colloidal particles. An important class of interparticle forces is induced by the presence of other colloidal species and arises solely as a result of entropic considerations. These entropic forces, or depletion forces, are strong enough to affect the behavior, both equilibrium and dynamic, of various dispersions of interest. For example, depletion forces are able to promote order-disorder transitions in the dispersion microstructure and may be responsible for a disorder-disorder transition. Passive structures etched into the walls of container can create entropic force fields of sufficient range and magnitude so that the motion and position of large colloids can be controlled. An understanding of these entropic forces has impact in materials processing, offering new mechanisms in which particles self-assemble in pre-chosen patterns or are sorted or organized along geometric features etched into a substrate for microfabrication.

We are currently developing theoretical and simulation methods to determine (1) the importance of entropic forces in affecting the stability, phase behavior, and particle deposition of dispersions and (2) the effectiveness of entropic forces as a mechanism for controlling the performance of dispersions. We are developing molecular theories that estimate entropic forces between particles and between particles and surfaces of various shapes. Such information provides the first step towards the prediction of the phase behavior and coagulation/deposition rates of dispersions. We are also investigating phase separations in colloidal dispersions using novel molecular simulation methods, determining both the compositions and structures of the equilibrium phases and the kinetics of the transitions. Simulation and analytical methods are also being employed to estimate the coagulation/

deposition rates of particles confined within various entropic force fields. This research will provide insights into the complex forces and phase behavior exhibited by colloidal dispersions, particularly for systems that are difficult to study with current experimental techniques. We are also exploring the novel use of entropic forces as a mechanism for the manufacture of new materials (e.g., nanomaterials and microelectronics).

Properties of Metastable Liquids; Molecular Theories of Nucleation
Metastable states arise, for example, when the temperature or pressure is changed from a value corresponding to a single, stable equilibrium phase to values corresponding to two phases in equilibrium. Instead of undergoing the equilibrium phase transition, the system remains in a one-phase metastable state. All phases of matter can exhibit metastability. Metastable liquids, in particular, are ubiquitous in nature, and have important technological applications. For example, superheated liquids (metastable with respect to the vapor phase) are important in maximizing yields during the rinsing and subsequent release of microelectromechanical devices after etching and in minimizing the erosion (via cavitation) of equipment in the chemical industry. The cyclic superheating of liquids with ultrasound is useful for cleaning surfaces, biological cell disruption, and the enhancement of chemical reaction and is important in the initial stages of sonoluminescence. In spite of their importance and widespread occurrence, fundamental questions persist about the properties of metastable liquids and their theoretical description.

We are studying both the equilibrium and kinetic properties of metastable systems using theoretical and molecular simulation methods. Molecular simulation studies of the thermophysical properties of superheated liquids are being performed in order to suggest ways in which van der Waals-like equations of state may be modified to provide a better description of the properties of superheated liquids. Molecular simulation methods will also be used to study stretched liquids confined between walls and to investigate how tensile strength changes under confinement. Another novel simulation approach focuses on local potential energy minima, called “inherent structures”, obtained by steepest-descent quenching of equilibrium configurations onto mechanically stable configurations in which the net force on each particle is zero. Simulations of the manner in which a system samples its potential energy surface or energy landscape have uncovered the importance of mechanically stable inherent structures in determining the properties of superheated liquids (including their tensile strengths). Inherent structures of superheated liquids are divided into a dense, amorphous phase and a void “phase” containing no atoms. Recent work analyzed the correlation between “weak spots” in the liquid (at high temperature) and the large voids formed in inherent structures (at absolute zero) demonstrating that atoms adjacent to large voids in the superheated liquid have a high probability of being found on the surface of the void “phase” in their corresponding inherent structures. This is a very important finding, as it establishes a direct correspondence between the appearance of large voids in superheated liquids and the sampling of suitable inherent structures. The analysis of inherent structures amounts to an entirely new way of looking at the kinetics of first-order phase transitions in liquids and should lead to an improved molecular-based understanding of bubble nucleation in superheated

liquids. In addition, since the appearance of voids in inherent structures is solely due to the attractive part of the intermolecular potential, this work also promises to improve our understanding of the mechanical failure of liquids and amorphous materials in the bulk and at interfaces.

Publications

D. S. Corti and H. Reiss, 1998, "Depletion Force Between a Colloid Particle and a Wall: Simple Theory by Means of Scaled Particle Theory," *Mol. Phys. 95*, 269-80.

B. Senger, P. Schaaf, D. S. Corti, R. Bowles, D. Pointu, J.-C. Voegel, and H. Reiss, 1999, "A Molecular Theory of the Homogeneous Nucleation Rate I: Formulation and Fundamental Issues," *J. Chem. Phys. 110*, 6421-37.

B. Senger, P. Schaaf, D. S. Corti, R. Bowles, D. Pointu, J.-C. Voegel, and H. Reiss, 1999, "A Molecular Theory of the Homogeneous Nucleation Rate II: Application to Argon Vapor," *J. Chem. Phys. 110*, 6438-50.

D. S. Corti and R. K. Bowles, 1999, "Statistical Geometry of Hard Sphere Systems: Exact Relations for Additive and Nonadditive Mixtures,'' *Mol. Phys. 96*, 1623-1635.

D. S. Corti, submitted, 1999, "Monte Carlo Simulations in the Isothermal-Isobaric Ensemble: The Requirement of a `Shell' Molecule and Simulations of Small Systems."

Invited Lectures

D. S. Corti, "Statistical Geometry of Hard Sphere Systems: Depletion Force Between a Colloid Particle and a Wall," School of Chemical Engineering, Purdue University, West Lafayette, IN, September 1998.

D. S. Corti, "Statistical Geometry of Hard Sphere Systems: Depletion Forces in Colloidal Systems," Department of Chemical Engineering, Rose-Hulman Institute of Technology, Terre Haute, IN, October 1998.

Meeting Presentations

S.-J. Lee, G. A. Medvedev, J. M. Caruthers, and D. S. Corti, "Constitutive Model for Pressure-Volume-Temperature Behavior of Polymeric Glasses: The Effect of Density Fluctuations," AIChE Annual Meeting, Miami Beach, FL, November 1998.

D. S. Corti, "Monte Carlo Simulations in the Isothermal-Isobaric Ensemble: The Requirement of a 'Shell' Particle," AIChE Annual Meeting, Miami Beach, FL, November 1998.

D. S. Corti and H. Reiss, "Depletion Force Between a Colloid Particle And A Wall: Simple Theory By Means Of Scaled Particle Theory," AIChE Annual Meeting, Miami Beach, FL, November 1998.

D. S. Corti and R. K. Bowles, "Statistical Geometry of Hard Sphere Systems: Exact Relations for Additive and Nonadditive Mixtures," Midwest Thermodynamics and Statistical Mechanics Meeting, Detroit, MI, May 1999.

W. Nicholas Delgass

1974

Professor and Associate Head of the School

Degrees

BSE, Chemical Engineering, University of Michigan, 1964

BSE, Mathematics, University of Michigan, 1964

MS, Stanford University, 1966

PhD, Stanford University, 1969

Interests

Heterogeneous catalysis

Selective hydrogenation over Raney nickel

Partial oxidation - Epoxidation

Solid acid catalysts

NMR, XPS, FTIR

Research Areas

Epoxidation of Olefins over Promoted Silver and Gold Catalysts. Silver is unique among the elements in its ability to catalyze the reaction of oxygen with ethylene to form ethylene oxide (EO) rather than the thermodynamically preferred product, CO_2. Silver is also known to catalyze epoxidation of butadiene to 3,4 epoxy 1-butene (EpB). Cs promotes catalysis of both reactions, but optimum formulations for the two systems are quite different. Studies of effects of Cs on Agactivity are now being followed by transient isotopic switch experiments, in which sudden replacement of $^{16}O_2$ with $^{18}O_2$ during steady state reaction allows us to quantitatively evaluate kinetically different oxygen pools on the surface of and in the catalyst. Previous work has shown that subsurface oxygen is a key ingredient of selective EO catalysts. We are interested to know the role of surface and subsurface oxygen species in EpB catalysis. Most recent studies of silver systems also use Raman spectroscopy to probe the role of Cs, include steady state kinetic analysis of effects of promoters, and are examining promotion by Re, which enhances EO selectivity without the usual corresponding loss in rate.

Generally, olefins, such as propylene, with allylic hydrogens cannot be epoxidized selectively over silver. Propylene oxide (PO) must currently be made in a two step process. The recent literature has reported that addition of hydrogen to a propylene/oxygen stream over a TiO_2-promoted gold catalyst gives a surprisingly high selectivity to PO. We are examining these systems both kinetically and spectroscopically and are working with Professor Andres, whose nanoparticle synthesis methods are being used to maximize the gold-titania interfacial contact and thereby

maximize the rate of PO production. One focus of current work is the hypothesis that hydroperoxide is the selective intermediate.

Investigation of Spatially Patterned Catalytic Reactors. The theme of this collaborative work with Professor Ramkrishna is to enhance the performance of a primary reaction system by introducing an auxiliary reaction system catalyzed by a second catalyst. This enhancement may occur by alleviating an equilibrium constraint, removing a reaction inhibitor, "tuning" the reactant feed, or annihilating an environmentally hazardous by-product.

The broad objective is to experimentally and theoretically study catalytic reactors with various types of spatial patterns intended to improve reactor selectivity and conversion. The patterns of interest, identified by their characteristic length scales, and are: (1) a well-mixed bed comprised of composite pellets containing both functionalities, (2) a well-mixed discrete bed containing different types of pellets with distinct functionalities, and (3) a spatially segregated bed alternating between layers of each distinct catalyst. More specifically, we seek to evaluate when each type of pattern will be most advantageous while generating a general methodology for properly orchestrating a pattern.

A wide variety of calculations indicate that these spatial hold great potential for improving the performance of many reaction systems and, therefore, may be attractive alternatives to traditional configurations. Work is current underway to demonstrate the effects experimentally in a methane to ethylene to benzene process. A fundamental understanding of spatial patterns, and their interplay with symmetry-breaking phenomena, may provide an avenue for greater optimization of dual-functional reactors thus maximizing conversion and selectivity to desired products or minimizing the production of hazardous by-products.

Selective Hydrogenation over Raney® Nickel. Caustic leaching of Al from an Al rich aluminum-nickel alloy produces a porous, high surface area nickel powder that is so reactive it is pyrophoric. Called Raney® nickel after its inventor, this material is a well-established catalyst for liquid phase hydrogenations. While the high activity is driven primarily by the high nickel surface area, residual aluminum, and promoters such as Fe, Cr, and Mo, play a role in controlling selectivity that is not yet understood. In this collaborative project with DuPont, we are studying the effects of alloy preparation and surface composition on the selective hydrogenation of butyronitrile and mesityl oxide. Reactions in methanol solution at pressures from 15 to 250 psig of hydrogen are being used to test effects of alloy composition (including new $NiMn_x$ materials), annealing, leaching and post-activation promotion on activity and selectivity. We collaborate with Professors Trumble and Gaskell in Materials Engineering on the production of the alloys, control of the grain size and phase distribution, and details of the leaching process.

Acid Zeolite Catalyzed Dehydration of 2,3 Butanediol to Methyl Ethyl Ketone. Work in Professor Tsao's laboratory has shown that a variety of hexoses and pentoses can be efficiently converted to 2, 3 butanediol biochemically. Dehydration of the diol to MEK completes the cycle to produce a useful commercial solvent from renewable resources. In collaboration with Professor Grutzner in Chemistry, we are studying a variety of zeolites with different pore structures, acidity, and acid site density to learn how to optimize these solid acid catalysts

for the dehydration reaction. Diffuse reflectance infrared spectroscopy (DRIFTS) is used to study the interaction between the diol and the zeolite surface. The combination of spectroscopic and kinetic measurements suggests that zeolite structure is important to activity, but that desorption of MEK can be the controlling step. The MFI structures which do facile dehydration at low temperatures can be too active, initiating aldol condensation and aromatization before the MEK desorption temperature is reached. Lessons learned from these systems will be applied to other opportunities to replace liquid acids by solid acid catalysts.

Publications

Thomas-Pryor, S. N., T. A. Manz, Z. Liu, T. A. Koch, S. K. Sengupta, and W. N. Delgass, "Selective Hydrogenation of Butyronitrile over Promoted Raney® Nickel Catalysts," *in Catalysis of Organic Reactions*, Frank Herkes, ed, Marcel Dekker (1998) 195-206.

J. W. Niemantsverdriet and W.N. Delgass, "In situ Mössbauer Spectroscopy in Catalysis." *Topics in Catalysis*, *8*, 133-140 (1998).

M. V. Badani and W. N. Delgass, "The Active Phase of Iron Catalysts for Acetonitrile Synthesis," *J. Catal.*, in press.

E. E. Stangland, K. B. Stavens, R. P. Andres, and W. N. Delgass, "Characterization of gold-Titania Catalysts via Oxidation of Propylene to Propylene Oxide," *J. Catal.*, submitted.

E. E. Stangland, K. B. Stavens, R. P. Andres, and W. N. Delgass, "Proplyene Epoxidation over Gold-Titania Catalysts," Proceedings of the 12th International Congress on Catalysis, Granada Spain (2000), submitted.

J. Lee, J. B. Grutzner, W. E. Walters, and W. N. Delgass, "The Conversion of 2, 3-Butanediol to Methyl Ethyl Ketone over Zeolites," Proceedings of the 12th International Congress on Catalysis, Granada Spain (2000), submitted.

Meeting Presentations

"Selective Hydrogenation over Raney® Nickel," Department of Chemical Engineering, Bogazici University, Istanbul, Turkey, October 8, 1998.

"Epoxidation of Propylene over Au/TiO_2 Catalysts," Seminar to Catalysis Group, Pennsylvania State University, University Park, PA, April 15, 1999

"Dehydration of Butanediol over Zeolite Catalysts," Philadelphia Catalylsis Club Spring Symposium in honor of Werner Haag, April 28, 1999

Roger E. Eckert

1964

Professor

Degrees

BS, Princeton University, 1948

MS, University of Illinois, 1949

PhD, University of Illinois, 1951

Interests

Statistical design of experiments

Flow properties of viscoelastic polymers

Mass transfer effect on reaction selectivity

Research Areas

Designing Experiments for Model Discrimination and Precise Parameter Estimation. One of the objectives of our research is to design experiments which give maximum information on the choice between models based on alternative mechanisms. A method has been developed which, in comparison with earlier work, leads more reliably to selection of the preferred model in fewer experiments.

The design of experiments for determining the validity of terms in *linear* models and for evaluating their parameters is well advanced and formalized. In the case of *nonlinear* models only the techniques for estimating the parameters have received much attention. Selection of experiments which give maximum information on the choice between alternative models has been combined with precise parameter estimation. The technique requires a number of experimental observations greater than the maximum number of parameters to be estimated in any of the models before the method can be initiated. In contrast, we have devised criteria to design the first and all subsequent experiments. Model discrimination is emphasized for the earlier experiments and gradually the emphasis switches to precise parameter estimation. In comparison with the published examples of the previous technique for sequential design of experiments for the purposes of discrimination and estimation, this improved method reaches a probability of virtually one for the preferred model in fewer experiments and also exceeds the others in the precision of the estimated parameters.

Applications of these principles and the developed computer program to other systems both in the field of kinetics, fluid flow, rheology, and other topics of chemical engineering should further demonstrate its value and general utility.

Applications of Statistics in Designing Experiments and Model Building for Complex Chemical Engineering Systems. Currently, sta-

tistical nonlinear modeling methods are being applied to clarify the chemical and physical phenomena during the alkylation of isobutane with light olefins. The size of dispersed droplets of organic phase in a variety of used sulfuric acid catalysts for the alkylation reaction is modeled for dependence on the physical properties of components and the intensity of agitation.

Polymer Flow Properties at High Shear Rates. Flow properties of viscoelastic polymers are being measured in novel and standard equipment with the ultimate objective of predicting those properties from chemical and physical structure. Emphasis is on the use of continuous flow devices with channels approximating infinite parallel plates to yield data in the industrially and fundamentally important *high shear rate region*. Additional measurements of the thrust of the emerging jet of polymer plus properties at low shear rates determined with a rheogoniometer lead to fundamental understanding of polymer flow. This information is valuable in designing equipment for processing polymers, for example extruders and textile fiber spinning systems.

Traditionally in flow-type rheometers, the flow was assumed viscometric up to the exit plane. If inertial effects are negligible, the primary normal stress difference can be obtained by extrapolating the pressure gradient to the exit. However, the purpose of such a calculation should be clearly understood. It is not to obtain the pressure at the exit, but the “extra pressure” existing throughout the channel because of the transverse normal stress. Both experimental data and calculational evidence show that as a viscoelastic fluid approaches the exit of a confined channel, the fluid accelerates near the wall and decelerates in the channel center. Velocity rearrangement occurs because the fluid goes from a simple shear flow to a shear-free one. Our specific interest is to model from experimental data any contribution that arrangement inside the channel makes toward measured properties.

Publications

Albright, L.F. and R.E. Eckert, "New and More Rapid Methods to Determine Octane Numbers of Alkylates Produced in Refineries," *Oil & Gas J.*, *97*, No. 3, 51-54, (Jan. 1999).

Elias I. Franses

1979

Professor

Degrees

Dipl. Eng., National Technical University, Athens, 1974

PhD, University of Minnesota, 1979

Interests

Interfacial Engineering - Thin Films - Mass Transfer

Adsorption and Tension Equilibria and Dynamics of Surfactants and Proteins at Interfaces

Adsorption and Transport of Lung Surfactants

Effects of Processing on Properties of Thin Organic Coatings

Transport and Ion Exchange in Thin Organic Langmuir-Blodgett and Spin-Coated Films

Infrared Spectroscopy, Ellipsometry, and Radiotracer Studies of Monolayers and Multilayers of Surfactants, Lipids, Proteins, and Polymer Films

Research Areas

Equilibrium Adsorption and Tension of Aqueous Surfactant and Lipids. Binary and multicomponent adsorption at air / water, oil / water, and liquid / solid interfaces and tension at fluid interfaces, are important factors in foam stability, emulsion stability, detergency, and coating flows, and lung surfactants function in the lung alveoli. Our main goals are to describe and predict competitive adsorption of nonionic or ionic surfactant mixtures from the surface behavior of the single surfactants and their mixing characteristics at the interface and in the bulk solution. We have been using the ideal or nonideal adsorbed solution models as our framework. For nonionic surfactant mixtures, we have developed such models and successfully tested them experimentally. We developed the first complete model to describe and predict tension and adsorption synergism, below and above the cmc (critical micellization concentration). The work is being extended to ionic surfactants, such as salts of fatty acids, where electrostatic effects are dominant (with A.J. Prosser). In addition, the equilibrium adsorption and spread monolayer isotherm of sparingly soluble higher alcohols is studied for determining the effect of their solubility and volatility on their surface tension behavior, and for their potential applications as ingredients of lung surfactant replacement drugs (with S.H. Myrick). Finally, with our Barcelona, Spain, collaborators (A. Pinazo, L. Perez, and M.R. Infante), we are studying the physical chemistry of new nonionic or gemini (two head groups, two tail groups) ionic surfactants they synthesized in Spain.

Our goals are to probe directly the surface composition, stability, and microstructure of these monolayers using radiotracer, optical, and infrared spectroscopic probes.

Dynamic Adsorption and Tension of Aqueous Surfactants, Lipids, or Proteins. Fast processes such as foaming, cleaning, coating flows, and breathing are affected more by the dynamic than by the equilibrium behavior. We have been using primarily the bubble method for measuring dynamic surface tensions at constant area or at pulsating area. Our new models and data at constant area revealed cases of dynamic synergism, where the mixture of surfactants has superior performance than either of the individual components at the same total concentration. We have been seeking for new molecules or systems which can reduce the dynamic tension under pulsating area to below 10 or 5 mN/m, which are called "superlow tensions," and are major requirement for lung surfactant replacement drugs (there are, of course, many biophysical and other requirements as well). We and others have found that compressed monolayers of a very select group of lipids or lipid/protein mixtures can produce superlow tensions. We have also discovered with (X. Wen and K.C. McGinnis) that dilauroylphosphatidylcholine and sodium myristate can also produce very low tensions. In our present and future research, we aim at understanding the key thermodynamic, dynamic (mass transfer and adsorption/desorption), colloidal, and molecular factors responsible for good (or poor) dynamic tension behavior. Direct optical and spectroscopic methods, primarily ellipsometry and reflection, absorption infrared spectroscopy, are also being used or further developed probing the interface and helping our model development and search for the most effective molecules.

With Prof. G. Narsimhan, in the School of Agricultural and Biological Engineering, and Dr. D. Cho, we have studied the adsorption/tension behavior of Bovine Serum Albumin, as a model globular protein, alone with a lipid. The goal is to understand the factors affecting foam-based separation method and foam stability in food products. We have developed models for diffusion of the protein to and from the surface layer, and are using a radiotracer method to directly measure the surface concentrations and stability of protein and surfactant monolayers.

Production and Characterization of Ultrathin Organic Films. Ultrathin films are important in microlithography, membranes barrier materials, sensors, and nonlinear optical materials. We are studying the thickness, thickness uniformity, and transport properties (to water) of films (0.002 - 2 mm) produced with the spin coating or Langmuir-Blodgett methods (with C.B. Walsh). Spinning speed, polymer concentration, and surface wettability are some of the important factors affecting film quality. Ellipsometry, at multiple angles and wavelengths, and FTIR spectroscopy are the main methods used for characterizing such films and also adsorbed or spread monolayers at the air/liquid interface.

Publications

Wen, X., McGinnis, K.C., and Franses, E.I., "Unusually Low Dynamic Surface Tensions of Aqueous Solutions of Sodium Myristate," *Colloids Surfaces A, 143*, 373-380 (1998).

Myrick, S.H., and Franses, E.I., "Effect of Chain Length on Equilibrium and Dynamic Surface Tension of Spread Monolayers of Aqueous Alcohols,"*Colloids Surfaces A*, *143*, 503-515 (1998).

Walsh, C.B., and Franses, E.I., "Thickness and Quality of Spin-Coated Polymer Films by Two-Angle Ellipsometry," *Thin Solid Films*, in press (1999).

Myrick, S.H., and Franses, E.I., "Effect of Dispersed Tetradecanol Particles or Droplets on the Dynamic Surface Tension of Aqueous Tetradecanol Systems," *Langmuir, 15*, 1556-1561 (1999).

Park, S.Y., Hannemann, R.E., and Franses, E.I., "Dynamic Tension and Adsorption Behavior of Aqueous Lung Surfactants," *Colloids Surfaces B*, accepted (1999).

Pinazo, A., Wen, X., Pérez, L., Infante, M.-R., and Franses, E.I., "Aggregation Behavior in Water of Monomeric and Gemini Cationic Surfactants Derived from Arginine," *Langmuir, 15*, 3134-3142 (1999).

Park, S.-Y., Baatz, J.E., Hannemann, R.E., and Franses, E.I., "Dynamic Surface Tension of Aqueous Dispersions of SP-C and DPPC, and Their Monolayer Behavior," special volume in honor of Prof. D.T. Wasan, *Emulsions, Foams, and Thin Films*, accepted (1999).

Meeting Presentations

AIChE Annual Meeting, Miami Beach, Florida, November 1998, "Effects of Hydrolysis on the Solution, Phase, and Tension Behavior of Aqueous Sodium Myristate," with X. Wen, presented by X. Wen.

AIChE Annual Meeting, Miami Beach, Florida, November 1998, "Effect of Dispersed Tetradecanol Particles or Droplets on the Dynamic Surface Tension of Aqueous Tetradecanol Systems," with S.H. Myrick, presented by S.H. Myrick.

AIChE Annual Meeting, Miami Beach, Florida, November 1998, "Novel Gemini Cationic Surfactants: Evidence of Uncommon and Complex Aggregation Behavior," with X. Wen, A. Pinazo, L. Perez, and M.-R. Infante.

AIChE Annual Meeting, Miami Beach, Florida, November 1998, "Thickness and Quality of Spin-Coated Polymer Films by Two-Angle Ellipsometry," with C.B. Walsh.

Robert A. Greenkorn

1965

R. Games Slayter Distinguished Professor of Chemical Engineering

Special Assistant to the President and Vice President for Special Programs of the Purdue Research Foundation

Degrees

BS, University of Wisconsin, 1954

MS, University of Wisconsin, 1955

PhD, University of Wisconsin, 1957

Interests

Flow phenomena in porous media

Pollution prevention

System modeling

Awards and Major Appointments

Editorial Board, *Transport in Porous Media*

Member of Board of Directors, Midwest Universities Consortium for International Activities (MUCIA)

Member of the University Corporation for Atmospheric Research (UCAR)

Research Coordinator for the Clean Manufacturing and Safe Materials Institute

Director, Purdue Technical Assistance Program

Research Areas

Magnetic Resonance Imaging of Mixing During Flow in Heterogeneous Porous Media. The displacement of pollutants in soils and underground reservoirs is a promising method for environmental restoration. A key technical challenge is to calculate the motion of the displacing fluid, the polluted fluid, and the mixing region between the two in heterogeneous porous media. Any biological remediation strategy requires statistical knowledge of the velocity covariance for both chemicals and bacteria. This information is also required to test the accuracy of modern theories of dispersion, such as nonlocal constitutive models. MRI micro-imaging techniques can be used to measure directly andnon-invasively, at a resolution of 10-500 microns, velocity covariance and concentration-time data. These measurements can be used to evaluate critically realistic non-local transport models for transport in heterogeneous porous media. The goal of this research is to explain mixing mechanisms in terms of the velocity variations and concentration of the displacing fluid and suspended particles as they flow through aperiodic heterogeneous adsorbing porous media.

System Modelling - A Model of University Enrollment, Research, Classes and Costs. Currently, four linear models have been constructed

for enrollment, research, classes and costs at Purdue University. These are being combined into a model system. Each department of the university is modeled. The models will be enlarged to include classes at six levels (freshman, sophomore, junior, senior, dual level and graduate classes) and by lecture, recitation, and laboratory.

Publications

Irwin, N.C., Greenkorn, R.A., Cushman, J.H. and Altobelli, S.A., 1999. "Magnetic Resonance Imaging Experiments for Examination of solutions to Stochastic Transport Problem of Order σ_v^N," *A.I.ChEJ.*, in press.

Irwin, N.C., Altobelli, S.A. and Greenkorn, R.A., 1999. "Concentration and Velocity Field Measurements by Magnetic Resonance Imaging in Aperiodic Heterogeneous Porous Media," *Mag. Res. Imag.*, in press.

Kuo, R.-K.H., Irwin, N.C. and Greenkorn, R.A., 1999. "Experimental Investigation of Mixing in Aperiodic Heterogeneous Porous Media: Comparison with Stochastic Transport Theory," *Trans. P.M.*, in press.

Irwin, N.C., Altobelli, S.A., Cushman, J.H., and Greenkorn, R.A., 1998 "NMR Imaging Experiments for Verification of Stochastic Transport Theory," *Mag. Res. Imag. 16* (5/6) 493.

Robert E. Hannemann

1969

Visiting Professor

Degrees

BSCHE, Purdue University, 1952

MD, Indiana University, 1959

Interests

Engineering in medical research and practice

Aerosols in medical practice

Lung surfactant – basic research and use in the treatment of the respiratory distress syndrome in infants

Non-invasive diagnostic techniques

Serum bilirubin and hemoglobin determination by skin reflectance

Awards and Major Appointments

Co-chair of Low Birth Weight Subcommittee of the Secretary's

(Health and Human Services) Advisory Committee on Infant Mortality

Visiting Professor - Biomedical Engineering Department

Research Areas

Aerosols in medical practice. This research is in the preliminary investigative phase. Current goal is aerosolization of lung surfactant for administration to infants with respiratory distress syndrome.

Surfactants in respiratory distress syndrome treatment. This research is being done in conjunction with Professor Elias Franses and is directed at understanding the basic processes associated with the action of lung surfactant.

Non-invasive diagnostic techniques. This research is in the preliminary investigative stage. Initial goal is the determination of the status of those techniques currently available and their applicability to the pre-natal, perinatal, newborn and infant stages of development.

Hemoglobin and serum bilirubin determination by skin reflectance. This research is being done in conjunction with Professors DeWitt and Xu (Mechanical Engineering).

R. Neal Houze

1969

Professor and Director of the Cooperative Education Program

Degrees

BS, Georgia Institute of Technology, 1960

MS, University of Houston, 1966

PhD, University of Houston, 1968

Interests

Interphase Mass Transfer

Free Boundary Turbulence

Awards and Major Appointments

Chairman of *Awards Committee*, Cooperative Education Division, American Society for Engineering Education

Member, *Clement J. Freund Award Committee,* American Society for Engineering Education

David P. Kessler

1964

Professor and Head, Division of Interdisciplinary Engineering Studies

Degrees

BS, Purdue University, 1956

MS, University of Michigan, 1959

PhD, University of Michigan, 1962

Interests

Transport in disperse media

Biomedical models

Book

Kessler, D.P., and Greenkorn, R.A. *Momentum, Heat, and Mass Transfer Fundamentals*, Marcel Dekker (1999).

Jochen A. Lauterbach

1996

Assistant Professor

Degrees

Dipl. - Phys., University of Bayreuth, Germany, 1992

Dr. rer. nat., Free University of Berlin, Germany, 1994

Interests

Surface chemistry and heterogeneous catalysis

Laser light based microscopy and spectroscopy

Time-resolved IR vibrational spectroscopy

Non-linear phenomena in catalysis

Low temperature oxidation catalysts

Polymer - metal interfaces

Combinatorial catalysis

Ultra-thin polymer films on metal and semiconductor surfaces

Awards and Major Appointments

Faculty Early Career Development Award (CAREER) from National Science Foundation

Research Areas

Many chemical processes involving surfaces, such as heterogeneously catalyzed reactions, semiconductor etching, or coating can be spatially inhomogeneous. This fact, however, is often neglected simply because no suitable microscopic tools are available to follow those processes in situ. To gain full understanding and control of the temporal and spatial dynamics, it is mandatory to employ both spectroscopy and microscopy techniques, preferably simultaneously. The long-term objective of our research is to study problems in heterogeneous catalysis and photopolymerization onto metal surfaces using novel surface imaging methods. Those techniques are combined with traditional vibrational and non-linear optics spectroscopy methods to perform in situ experiments in the following two research areas.

Non-linear phenomena in heterogeneous catalysis. Synergetic effects on very different length scales are among the most fascinating phenomena nature can create. During the past two decades, scientists and engineers from many disciplines have become increasingly interested in oscillations, multiple steady states, spatial structures, and wave propagation occurring in chemical, biochemical, and biological systems. Heterogeneously catalyzed reactions serve as model systems where pattern formation is restricted to two dimensions on the catalyst surface. Preparation of the catalyst under well-defined ultra-high vacuum conditions provides a

deeper understanding of the fundamental properties of the non-linear phenomena observed for many technologically and environmentally important reactions. Reactions are considered to be isothermal in the lit superior performance. The expectation that the catalytic behavior of two active materials is additive is simply not valid. Using microcomposite model surfaces produced via microlithography, we investigate how areas on the catalyst with different activity couple and determine the overall behavior of the catalyst.

In addition to the experimental research, simulations of the observed non-linear phenomena are performed using reaction-diffusion models. Building on our experimental results, the models are expanded to include gas-phase coupling and non-isothermal phenomena. This requires, for example, the addition of heat transfer in the catalyst and fluid phase. Comparison with our experimental data for the high pressure regime will improve the existing models and will lead to a better understanding of heterogeneously catalyzed reactions under realistic pressure conditions.

Surface Chemistry of Polymer-Metal interfaces. The second area of applications of in situ, light based techniques applies the surface science approach to the investigation of polymer-metal surface interactions. One of the most exciting aspects in this field is the understanding of the interface between a polymer and a solid or a gas, and the consequent changes in the electronic, thermodynamic and structural behavior in comparison with those of the bulk polymer. These effects are maximal in the first monolayer of the interfacial region. Such polymeric monolayers, particularly when possessing a high degree of two-dimensional order, are of importance from the point of view of both technological development and fundamental research. To cite a couple of instances; microelectronics demands size-reduction of components, and the quasi-one-dimensional behavior of ordered monolayers is of interest in fundamental research. Direct photopolymerization reactions are extremely important for a variety of coating and device applications such as corrosion resistance and electric insulation. We combine investigations at pressures in the Torr range, performed in a polymer reactor, with UHV adsorption and monolayer polymerization studies to analyze the surface chemistry of the polymer-metal interaction. We are using time-resolved FTIR spectroscopy for in situ characterization adsorption and photopolymerization of acrolein, methacrolein, and styrene on a variety of transition metal surfaces. The objective of this project is to elucidate the adsorption kinetics of the monomer and the polymerization dynamics. Two possible processes are gas-phase polymerization and subsequent adsorption of the formed polymer on the metal surface versus adsorption of the monomer and polymerization on the surface. Information about polymer layer thickness can be obtained with EMSI, in particular if performed with FTIR simultaneously. The focus of this application of EMSI is on the adsorption of monomers on a variety of well-defined metal surfaces and the effects of different underlying metal substrates on the photopolymerization process. Comparing different metals enables us to draw conclusions about the influence of the surface electronic and geometric structure on the polymer formation process.

Combinatorial catalysis. Combinatorial technologies have generated much scientific excitement in the past few years because they maximize the opportunity for methodical breakthroughs and expand the amount of available information. The underlying principle is to synthesize small

quantities of a compound, and to scan them quickly in libraries to make well-informed decisions and to find unexpected trends. The two main challenges are the controlled synthesis of small amounts of materials and the parallel analysis of libraries of these materials, for which new high-throughput analytical screening techniques need to be invented. We have developed a novel system for spatially resolved measurements of the IR absorption by molecular vibrations in combinatorial libraries, allowing for in situ parallel studies of catalyst libraries, liquid-phase and solid surface reactions, and traditional bead-based combinatorial systems. This novel analytical technique, based on FTIR spectroscopy, has many advantages over currently available technology by performing parallel analyses of entire solid-phase combinatorial libraries in a matter of minutes. Studies are currently performed for heterogeneous catalysts and solid-phase combinatorial bead libraries.

Design of novel and improved catalysts requires an understanding of the mechanism of the catalytic reaction and knowledge of the properties that determine activity, selectivity, and lifetime of the catalyst. Studies of the interrelationship between structural and chemical properties of solid materials and their catalytic properties are at the beginning of catalyst design. The search for effective heterogeneous catalysts is often a lengthy process, where different catalytic materials are tested one at a time in single model reactors. Our goal is to correlate fundamental reaction mechanisms with activity by simultaneous investigation of libraries of catalysts in a single reactor. Combinatorial libraries with catalyst micro-samples contain supported catalysis with different metal loading. Libraries are placed in a small flow reactor. The main emphasis is to elucidate fundamental reaction mechanisms as a function of catalyst composition by following adsorbates in situ under reaction conditions. We focus on mechanistic studies using the imaging IR system, and correlate the IR vibrational results with the chemical composition of the library elements. Promising catalyst compositions are then further tested and improved using traditional methods of catalysis research. We test new catalyst compositions for decomposition of NO as well as NO reduction via hydrocarbons as a reducing agent. These catalysts are based on rhodium, palladium and other platinum group metals mixed with additives, such as rare earth elements. Mechanistic combinatorial studies provide us with systematic trends about adsorbed species and reaction intermediates as a function of the catalyst composition and reaction conditions. Isotopic mixing experiments help to assign IR absorption bands of the adsorbed species. Reactions are performed under a variety of conditions (reactant composition, total pressure in the reactor, catalyst temperature) to learn more about trends in adsorbed species as a function of catalyst composition. The possibility of systematically covering a very wide area of catalyst compositions helps us to identify new and improved catalyst systems and also leads to the optimization of present rhodium based systems.

Publications

T.A. Jachimowski and J. Lauterbach, “A combined pressure reaction cell–UHV chamber with sample transfer system," *Review of Scientific Instruments, 69(7);* 2757-2761, 1998.

G. Bonilla, T.D. Pletcher, G. Haas, and J. Lauterbach, “Unsteady-state behavior of CO oxidation over a supported Pt catalyst in the Torr range," *Reaction Kinetics and Catalysis Letters, 65(1)*; 3-8, 1998.

J. Lauterbach, K. Asakura, P.B. Rasmussen, H.H. Rotermund, M. Bär, M.D. Graham, I.G. Kevrekidis, and G. Ertl, “Catalysis on mesoscopic composite surfaces: Influence of palladium boundaries on patter formation during CO oxidation on Pt(110)," *Physica D - Nonlinear Phenomena, 123*; 493-501, 1998.

T. Lee, J. Liu, D.B. Janes, V.R. Kolagunta, J. Dicke, M.R. Melloch, D. McInturff, J.M. Woodall, R.P. Andres, J. Lauterbach, and R. Reifenberger, “An Ohmic NanoContact to GaAs," *Applied Physics Letters, 74(19)*; 2869-2871, 1999.

J. Lauterbach, G. Bonilla, and T.D. Pletcher, and, “Unsteady-state behavior of CO oxidation over supported Pt catalysts and Pt single crystals: A comparison in the Torr pressure range," *Chemical Engineering Science, 54(20)*; 4501-4512, 1999.

K. Green, T.A. Jachimowski, and J. Lauterbach, “The adsorption and photopolymerization of methyl methacrylate on Pt(110)," *Surface Science*, submitted, 1999.

D.B. Janes, R.P. Andres, M. Batistuta, E.H. Chen, J. Dicke, V.R. Kolagunta, J. Lauterbach, T. Lee, J. Liu, M.R. Melloch, E.L. Peckham, T.D. Pletcher, R. Reifenberger, H.U. Ueng, B.L. Walsh, J.M. Woodall, C.K. Kubiak, and B. Kasibhatla, “Nanoelectronic device applications of a chemically stable GaAs structure," *Journal of Vacuum Science and Technology B, 17; 1773-1777*, 1999.

J. Dicke, H.H. Rotermund, and J. Lauterbach, “Ellipsomicroscopy for surface imaging: contrast mechanism and applications," *Journal of the American Optical Society A: Optics, Image Science, and Vision*, in press, 1999.

J. Dicke and J. Lauterbach, "Formation of a new oxygen species on Pt(100) during CO oxidation," *Surface Science*, in press, 1999.

Invited Lectures

J. Lauterbach, “Non-linear phenomena in catalysis," presented at the Chemical Engineering Department, University of Houston, TX, October 1998.

J. Lauterbach, “Non-linear phenomena in heterogeneously and homogeneously catalyzed reactions," presented at the Fritz-Haber-Institut, Berlin, January 1999.

J. Lauterbach, “ Imaging non-linear phenomena in surface reactions: the CO oxidation on platinum," presented at the Chemical Engineering Department, University of Louisville, KY, April 1999.

Meeting Presentations

G. Bonilla, T.D, Pletcher, G. Haas, and J. Lauterbach, “Unsteady behavior of CO oxidation over Pt catalysts: self-sustained rate oscillations in the Torr pressure range," at GEM meeting, Miami, FL, July 1998.

T.D, Pletcher and J. Lauterbach, “Spatio-temporal pattern Formation During the CO oxidation on Pt(100) in the mTorr pressure range," presented at the fall meeting of the Prairie Chapter of the American Vacuum Society, Argonne National Lab, Chicago, Il, September 1998.

J. Yan, K. Green, T. Jachimowski, and J. Lauterbach, “UV Photo-polymerization of Methyl Methacrylate and Acrylic Acid on Pt(110) Using Time-Resolved FT-IRAS," presented at the fall meeting of the Prairie

Chapter of the American Vacuum Society, Argonne National Lab, Chicago, Il, September 1998 [won 2nd prize in student poster competition].

J. Yan, K. Green, T. Jachimowski, and J. Lauterbach, “UV Photo-polymerization of Methyl Methacrylate and Acrylic Acid on Pt(110) Using Time-Resolved FT-IRAS," presented at the fall meeting of the American Vacuum Society, Baltimore, MD, October 1998.

J. Right, G. Bonilla, T.D. Pletcher, and J. Lauterbach, “Unsteady Behavior of CO Oxidation on Platinum Single Crystals and Supported Catalysts," AIChE North Central Region representative at the National Student Paper of AIChE, Miami, FL, November 1998.

G. Bonilla, T.D. Pletcher, and J. Lauterbach, “Unsteady Behavior Of CO Oxidation Over Supported Pt Catalysts And Pt(100)," Fall meeting of AIChE, Miami, FL, November 1998.

G. Bonilla, T.D, Pletcher, G. Haas, and J. Lauterbach, “Unsteady behavior of CO oxidation over supported Pt catalysts and Pt single crystals: self-sustained rate oscillations in the Torr pressure range," presented at the fall meeting of AIChE, Miami, FL, November 1998.

N. Saadah, T. Beutien, B. Ecker, H. Grinstead, C. Forthoffer, J. Ralston, A. Schreiweis, and J. Lauterbach, “Chemical Reactions in Microgravity," presented at the annual meeting of the American Astronautics Society (AAS) Houston, TX, November 1998.

J. Dicke and J. Lauterbach, “EMSI and RAM: Two novel optical techniques used to image spatio-temporal pattern formation during CO oxidation on Pt at elevated pressures," presented at the GORDON Research Conference, Ventura, CA, February 1999.

B. Walsh, D.B. Janes, E. Peckham, Q. Qu, M. Batistuta, J. Lauterbach, and M.R. Melloch, “Micro-contact patterning of GaAs using a self-assembled monolayer resist," presented at the centennial meeting of the American Physical Society, Atlanta, GA, March 1999.

J. Dicke, T.D. Pletcher, and J. Lauterbach, “EMSI and RAM: Two novel optical techniques to image ultra-thin layers," presented at the centennial meeting of the American Physical Society, Atlanta, GA, March 1999.

J. Lauterbach, “Spatio-temporal pattern formation during CO oxidation over Pt(100)," presented at GORDON Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Il Ciocco, Italy, June 1999.

C. Snively and J. Lauterbach, “A novel FTIR imaging system for parallel screening of combinatorial catalyst libraries," presented at the 1st NATO workshop on Combinatorial Catalysis, Portugal, July 1999.

Jay H. Lee

1998

Associate Professor

Degrees

BS, University of Washington, 1986

PhD, California Institute of Technology, 1991

Interests

Model-Based Predictive Decision Making

Soft Sensor and Inferential Control

System Identification and Plant Experiment Design

Learning Control of Batch and Periodic Systems

Batch Recipe Generation, Scale-Up and Modification

Recovery from Abnormal Operational States

Awards and Major Appointments

National Science Foundation Young Investigator Award (1993-1999)

Research Areas

Model-Based Predictive Decision Making. Model-based predictive decision making refers to an optimization based framework wherein a system model and measurements are used together to predict the relevant system behavior within some future time horizon and the decision variables are optimized based on the prediction and some mathematical objective (involving an objective function and constraints). It has thus far seen its application primarily in control but has the potential to be applied to a number of other decision-making processes such as scheduling, resource management and other planning activities. In this research, we examine the similarities and differences among different candidate activities (in terms of their models, types of decision variables, frequency of information update, etc.) and develop general as well as activity-specific tools.

Soft Sensor and Inferential Control. In this research, we are attempting to arrive at a best methodology to fuse two most prominent computational techniques the information age has brought to the process industry, namely model-based predictive control and soft sensing ("virtual analyzers"). The motivation for combining the two is to control product properties that were not controlled (at least not tightly) traditionally. Motivated by the shortcomings of the current industrial practice of inferential control which combines the soft sensor with a regular feedback controller through a simple series connection, we pursue the alternative approach of model-based design. We examine the modeling requirement for this and develop theories and tools for it. We are also conducting a number of case studies involving multi-component distillation columns,

pulp digesters and polymer reactors. While our past efforts were centered on linear techniques, our current focus is on developing theories and tools for highly nonlinear systems.

System Identification and Experiment Design. Almost all model based control systems implemented today are designed based on data from plant tests. Plant tests are by far the most time consuming and costly step in an advanced control system commissioning, accounting for up to 90% of the cost and time. Hence, it is of interest to optimize the plant test procedure so that the information most needed for the intended closed-loop control can be extracted in a safe, efficient manner. While traditional approaches to optimal experimental design centered around the objective of minimizing some measure of parameter covariance matrix, we attempt to relate the parameter variance distribution directly to the end closed-loop objective, to formulate a "control-relevant" optimal design criterion. The developed method based on the criterion tries to take advantage of the ever increasing computational power so that more of practically important issues such as constraints and safety can be accounted for.

Learning Control of Batch and Periodic Systems. A unique aspect of batch systems is that the operation follows a periodic pattern. Besides batch processes, there are many continuous processes, such as pressure-swing adsorption systems and simulated moving-bed systems, that exhibit periodic behavior. Control technique that do not exploit the periodic nature of these processes lead to poor control results in general due to the nonstationary nature of the operation. In this research, we incorporate the concepts like "iterative learning control" and "repetitive control" into the framework of model-based predictive control to develop a control technique specifically tailored to exploit the periodic nature. The result is that run-to-run improvement and even complete convergence can be achieved as the periodic operation is repeated. Another interesting aspect of these process types is that they involve discrete as well as continuous state and decision variables, requiring a hybrid system description. Theories and tools are being developed and applied to a number of processes including polymer reactors, pressure-swing adsorption systems and simulated moving-bed systems.

Batch Recipe Generation, Scale-Up and Modification. Development of an industrial batch recipe often involves a painstaking series of trial-and-error runs, requiring substantial development time and resource. In addition, scaling up a recipe to a commercial production scale is not at all straightforward and gives rise to a long "learning period" wherein continuous modifications are made to achieve the full expected yield and product quality. Finally, due to disturbances and subtle ingredient changes, abiding to a fixed recipe seldom yields a product of consistent quality at the full potential yield. In this research, we are developing a systematic framework and associated methodologies and tools for generating a batch recipe, scaling it up and refining/modifying it during the real operation. Our approach is model-based and we attempt to integrate on-line and off-line data as well as qualitative and quantitative knowledge with the context of model building and model updating. Key techniques we employ are parameter sensitivity analysis, statistical modeling, optimal estimation and predictive control.

Recovery from Abnormal Operational States. Most industrial processes experience occasional abnormal periods during which the pro-

cess loses stability and the product variability shoots up. Causes for such abnormalities are known in many cases, as in the cases of utility problems or temporary process shutdowns, but there are those where the cause is unknown and requires a systematic diagnosis. Recovery from these abnormal states are often beyond the realm of conventional feedback control, as they require nonlinear system analysis and possibly a sequence of discrete actions. In this research, we are developing a methodology and tools to use a rigorous process model to compute an optimal strategy for recovery. The basic tools we employ are nonlinear state estimation and nonlinear predictive control. We acknowledge the impracticality of solving a full-scale nonlinear program on-line and address how we can utilize off-line computation to relieve the on-line computation.

Publications

Kesavan, P., J. H. Lee and A. Krishnagopalan, "PLS-based Control of Batch Pulp Digesters," *Journal of Process Control*, in press, 1999.

Amirthalingam, R. and J. H. Lee, "Inferential Control of Continuous Pulp Digester," *Journal of Process Control*, in press, 1999.

Russell, S., D. G. Robertson, J. H. Lee and B. Ogunnaike, "Model-Based Quality Monitoring of Batch and Semi-Batch Processes," *Journal of Process Control*, in press, 1998.

Morari, M. and J. H. Lee, "Model Predictive Control-Past, Present and Future," *Computers and Chemical Engineering*, in press, 1999.

Lee, J. H. and B. Cooley, "Stable Min-Max Control of State-Space Systems with Bounded Input Matrix," *Automatica*, in press, 1998.

Lee, J. H., K. S. Lee and W. C. Kim "Model-Based Iterative Learning Control with a Quadratic Criterion for Time-Varying Linear Systems," *Automatica*, accepted, 1999.

Lee, K. S., I. S. Chin and J. H. Lee, "A Model Predictive Control Technique for Batch Processes and Its Application to Temperature Tracking Control of An Experimental Reactor,"*AIChE J.*, accepted, 1999.

Chikkula, Y., J. H. Lee and B. Ogunnaike, "Dynamic Scheduled Model Predictive Control Using Hinging Hyperplane Models," *AIChE Journal, 44*, pp. 2658-2674, 1998.

Russell, S., P. Kesavan, J. H. Lee and B. Ogunnaike, "Recursive Data-Based Prediction and Control of Product Quality for Batch and Semi-Batch Processes Applied to a Nylon 6,6 Autoclave," *AIChE Journal*, *44*, pp. 2442-2564, 1998.

Russell, S., D. G. Robertson, J. H. Lee and B. Ogunnaike, "Quality Monitoring and Control of Nylon 6,6 Autoclave," *Chemical Engineering Science, 53*, pp. 3685-3702, 1998.

Cooley, B. and J. H. Lee, "Integrated Identification and Robust Control," *Journal of Process Control, 8*, pp. 431-440, 1998.

Lee, J. H., Y. Pan and S. Sung, "A Numerical-Projection-Based Approach to Nonlinear Model Reduction and Identification," Proc. of American Control Conference, San Diego, CA, pp. 1568-1372, 1999.

Dorsey, A. W. and J. H. Lee, "Subspace Identification for Batch Processes," *Proc. of American Control Conference*, San Diego, CA, pp. 2538-2542, 1999.

Rao, C., J. B. Rawlings and J. H. Lee, "Stability of Constrained Moving Horizon Estimation," Proc. of American Control Conference, San Diego, CA, pp. 3387-3391, 1999.

Lee, K. S. and J. H. Lee, "Design of Quadratic Criterion-based Iterative Learning Control," *Iterative Learning Control: Analysis, Design, Integration and Applications*, edited by Z. Bien and J. Xu, pp. 165-192, Kluwer Academic Publisher, Boston, MA, 1998.

Lee, K. S. and J. H. Lee, "Model-Based Predictive Control Combined with Iterative Learning for Batch or Repetitive Processes," *Iterative Learning Control: Analysis, Design, Integration and Applications*, edited by Z. Bien and J. Xu, pp. 313-334, Kluwer Academic Publisher, Boston, MA, 1998.

Cooley, B. and J. H. Lee, "Control-Relevant Experiment Design," *Automatica*, revised and submitted, 1998.

Lee, K. S. and J. H. Lee, "Convergence of Constrained Model-Based Predictive Control Technique for Batch Processes," *IEEE Transactions on Automatic Control*, revised and submitted, 1998.

Lee, J. H. and K. S. Lee, "Model Based Predictive Control Approaches to Iterative Learning /Repetitive Control of Batch Processes and Continuous Processes with Periodic Operations,"*International Journal of Control*, submitted, 1999.

Chin, I. S., K. S. Lee and J. H. Lee, "A Technique for Integrated Quality Control, Profile Control and Constraint Handling for Batch Processes," *Ind. Eng. Chem. Res*., submitted, 1999.

Kesavan, P. and J. H. Lee, "Selective, Intermittent Adaptive Control of Processes Subject to Large and Infrequent Changes," *Chemical Engineering Science*, submitted 1999.

Kesavan, P. and J. H. Lee, "A Set-Based Approach to Detection and Isolation of Faults in Multivariable Systems," *Computers and Chemical Engineering*, submitted, 1999.

Chikkula, Y. and J. H. Lee, "Robust Adaptive Predictive Control of Nonlinear Processes Using Input-Output Models," *Ind. Eng. Chem. Res.*, submitted, 1999.

Lee, Y., J. H. Lee and S. W. Park, "On Interfacing Model Predictive Controllers with Low-Level Loops," *Ind. Eng. Chem. Res.*, submitted, 1999.

Robertson, D. G. and J. H. Lee, "On the Use of Constraints in Least Squares Estimation and Control," *Automatica*, submitted, 1999.

Meeting Presentations

Lee, J. H., the discussant for the paper "Statistical Performance Monitoring of Industrial Control Loops" at Gordon Research Conference on Statistics, New Port, RI, 1998.

Lee, K. S. and J. H. Lee, "Integrated Quality Control, Profile Control and Contstraint Handling for Batch Processes," AIChE Annual Meeting, Miami Beach, FL, 1998.

Amirthalingam, R. and J. H. Lee, "A Two Step Procedure for Data-Based Design of Inferential Control System and Its Application to A Multi-Component Distillation Column," Miami Beach, FL, 1998.

Lee, J. H., Y. Pan and S. Sung, "A Numerical-Projection-Based Approach to Nonlinear Model Reduction and Identification," American Control Conference, San Diego, CA, 1999.

Dorsey, A. W. and J. H. Lee, "Subspace Identification for Batch Processes," American Control Conference, San Diego, CA, 1999.

Rao, C., J. B. Rawlings and J. H. Lee, "Stability of Constrained Moving Horizon Estimation," American Control Conference, San Diego, CA, 1999.

Invited Lectures

"Plant-Friendly, Optimal Test Signal Design for Control-Relevant System Identification," the keynote lecture, The 3rd Midwest Control Workshop, University of Illinois, Urbana, IL, May, 1999.

"Iterative Learning Control for Batch Chemical Processes," Iterative Learning Control Workshop, Tampa, FL, Dec. 1998.

Chaired Conferences and Symposia

Organized and chaired the session "Data-Based Approaches to Process Control," at 1998 AIChE Annual Meeting, Miami Beach, FL.

Organized and chaired the session "Nonlinear Model Reduction and Identification," at 1999 American Control Conference, San Diego, CA.

Selected as an Area Chair (for the Area of System Identification) for IFAC ADCHEM Symposium, Pisa, Italy, 2000.

Selected as the General Co-Chair for IFAC DYCOPS Symposium, Cheju Island, Korea, 2001.

Joseph F. Pekny

1990

Associate Professor

Degrees

BS, Princeton University, 1985

PhD, Carnegie-Mellon University, 1989

Interests

Process scheduling, planning, & design

Risk management

Product pipeline & project management

Combinatorial optimization

Algorithm engineering methods

Software engineering methods

Research Areas

Algorithm Engineering For Large Scale Manufacturing Optimization Problems. Continuing rapid advances in computing technology are fostering an information-rich environment as industry moves towards comprehensive enterprise-wide data systems. As such, manufacturing processes can be modeled in great detail and populated with real time data in order to optimize behavior over a range of time scales from scheduling, planning, and design / retrofit problems up through supply chain management. The result of these modeling efforts promises to be more efficient processes that use less raw material, produce less waste, keep smaller inventories, are more responsive to customer needs, and are more flexible in the event of a changing product / raw material slate. In the future, the potential exists for building interconnected and consistent models which permit optimizing company-wide resources over many alternative choices so that the best can be implemented in practice. The trend towards such a "virtual manufacturing network" is a manifestation of the fact that the economy is grounded on information flow and the ability to efficiently manage it. In mechanistic terms, models provide a framework by which various pieces of information can be related in a goal-oriented context. However, in order to realize the potential of the models comprising virtual manufacturing networks, one significant capability which must be developed is the ability to quickly solve the large scale optimization problems implied by the complex nature of integrated industrial processes. Thus, developing algorithms for highly structured and large-scale manufacturing optimization problems is a research challenge involving the interaction of process physics, computer science, and applied mathematics. The goal is to engineer algorithms which provide high quality answers using

reasonable computational resources inside robust and cost effective software systems that respond intuitively to user interaction.

Our research over the last several years has shown that the formalism of mixed integer linear programming (MILP) based models offers a unique combination of scalability and flexibility—the ability to extract answers of provable quality and the potential for significantly lower installation and maintenance costs relative to other modeling technologies. Within the MILP domain a number of research areas are critical to achieving more capable optimization algorithms. In particular, twentieth century mathematics has disproved the notion of generic solution algorithms that can capably address all complex problems of interest. Instead mathematical theory and practical experimentation suggests that special purpose algorithms, designed for narrow but important classes of problems, are the only means of obtaining the several order of magnitude performance boost necessary to make large-scale, model-based manufacturing optimization a reality. Our ultimate goal is to make the effort necessary to develop special purpose optimization algorithms much smaller. To this end, research is being conducted in physically motivated problem decomposition and primal heuristic methods, software engineering for large scale optimization tool boxes, and the interaction between problem formulation and solution algorithms. Because the ability to solve linear programs is crucial to solving MILP models, research is being conducted in dynamic and problem structure specific matrix factorization, primal-dual solution methodology, simplex algorithm pivot rules with a physical interpretation, and the integration of separation algorithms for implicitly detecting violated constraints with algorithms for their enforcement. Experience shows that mathematical programming methods provide a powerful superstructure in which to address details, however practical algorithms must incorporate expert system, pattern recognition, evolutionary programming methods, abstract data types, or other symbolic reasoning techniques that are used to exploit gross problem structure and enhance development and computational performance. Underlying the research in the modeling and solution of manufacturing optimization problems is the study of fundamental combinatorial optimization problems on which new technology can be prototyped and the results of which can be used as building blocks in the solution of practical industrial problems. For example network flow, matching, assignment, multiply constrained knapsack, and traveling salesman problems embody aspects of phenomena present in industrial process management.

Risk and Uncertainty in Process Management. Fundamental physics shows that uncertainty is an integral part of reality. At the macroscopic level this uncertainty manifests itself as an inability to measure quantities with arbitrary precision and unplanned events. In conjunction with complexity, uncertainty is a major impediment to the efficient management of process resources. An important means for coping with uncertainty is the development of risk management strategies that are effective over a large fraction of possible outcomes. The goal of our research is the formation and investigation of such strategies in the context of their deployment in process decision support systems. This research encompasses methods for incorporating uncertainty directly into optimization models, the development of systematic “what-if” paradigms, Mixed Integer Linear Programming (MILP) sensitivity analysis, parametric optimization, and risk analysis. A major goal of this research is the ability

to dynamically answer questions such as the following: how much inventory or idle capacity should be kept as an insurance policy, when should an order be promised for delivery to a customer, is external (third-party) contracting an attractive option, which types of contractual features are desirable with suppliers and customers to best match process physics, when should existing facilities be cannibalized for new production capacity instead of building facilities, and what will be the impact of implementing a proposed product? A natural outcome of this research is the ability to demarcate and respond to operational difficulties due to uncertainty, process complexity, and the interaction between the two phenomena. An important practical outcome of the proposed research will be quantitative and qualitative methods for making the risk and reward of options more intuitive and provide details as to the potential impact of uncertainty and how it propagates through process networks. This includes identifying management strategies that effectively are both cost-effective and provide adequate protection against the most damaging and/or the most likely uncertain events. Research shows that the best management strategies strongly depend on process details and must constantly be changed to reflect business and process conditions.

Management of the Research, Development, and Commercialization Pipeline. The research, development, and subsequent commercialization of new products presents several resource/capital management problems that are both combinatorial in nature and involve substantial uncertainties. Furthermore, the increasing necessary integration of business functions requires that manufacturing considerations also be addressed within the context of deploying new products. The goal of this research is to develop modeling technology applicable to the management of the research and development pipeline, the management of resources used to commercialize new products, and overall mechanistic models which encompass research and development, manufacturing, marketing, and their interrelationship. This approach must address several types of uncertainty which are manifested differently in mathematical models. For example, uncertainty due to demand usually arises in the objective function while uncertainty due to experimental product attrition arises in constraints. Thus strategies for handling different types of uncertainties must be fundamentally different and customized for a particular problem physics. Additional applications of the research include coordination of marketing promotions with manufacturing capability. The research also considers game theoretic uses of multiple models to treat the behavior of corporate competition.

Publications

B. Ramachandran and J. F. Pekny, "Lower Bounds for Nonlinear Assignment Problems Using Many Body Interactions," *European Journal of Operational Research, Vol. 105, No. 1,* pp. *202-215, 1998.*

M. Zentner, A. Elkamel, J. Pekny, and G. V. Reklaitis, "A Language for Describing Process Scheduling Problems," *Computers and Chemical Engineering, Vol. 22, No. 1-2,* pp. 125-145, 1998.

J.F. Pekny and G.V. Reklaitis, "Towards the Convergence of Theory and Practice: A Technology Guide for Scheduling/Planning Methodology," Foundations of Computer Aided Process Operations Conference Proceedings, invited paper, pp. 91-111, 1998.

J. F. Pekny and G. E. Blau (editors), "Proceedings of the Third International Conference on the Foundations of Computer-Aided Process Operations," *AIChE Symposium Series, No. 320*, Vol 94, 1998.

Meeting Presentations

J. F. Pekny, "A Practical Guide to Technology for Managing Process Operations," invited tutorial lecture, AIChE Spring National Meeting, 1998.

S. J. Honkomp, P. Basu, B. Houston, and J. Pekny, "Managing the Pharmaceutical Product Development Pipeline," AIChE Spring National Meeting, 1998.

Ö. Samikoglu, S.J. Honkomp, J.F. Pekny, and G.V. Reklaitis, "Sensitivity Analysis for Project Planning and Scheduling under Uncertain Completions," European Symposium on Computer Aided Process Engineering-8, 1998.

J. F. Pekny, "Using Advanced Planning and Scheduling Systems to Manage Change and Complexity," APICS: The American Society for Resource Management Process Industry Conference, Erie, Pennsylvania, 1998.

S. J. Honkomp, J. F. Pekny, G. V. Reklaitis, and D. Subramanian, "A Computational Architecture for Addressing Both Combinatorial and Stochastic Aspects of Process Management Problems," AIChE Fall National Meeting, 1998.

D. G. Gerogianni, J. F. Pekny, and G. V. Reklaits, "Exploiting Deterministic Methods in the Treatment of Risk Analysis for Process Management Problems: An Approach for Problems Exhibiting Knapsack Substructure," AIChE Fall National Meeting, 1998.

J. F. Pekny, "An Inductive Approach to Developing Mathematical Programming Based Approaches to Industrial Scale Planning and Scheduling Problems," Informs Spring Meeting, Cincinnati, 1999.

G. E. Applequist, J. F. Pekny, and G. V. Reklaitis, "Economic Risk Management for Design and Planning of Chemical Manufacturing Supply Chains," AIChE Fall National Meeting, 1999.

S. Bose, J. F. Pekny, and B. Ramachandran, "A Forecasting-Optimization-Simulation Based Approach to Consumer Goods Supply Chain Management Under Uncertainty," AIChE Fall National Meeting, 1999.

Nicholas A. Peppas

1976

Showalter Distinguished Professor of Biomedical Engineering

Degrees

DEng, National Technical University, Athens, 1971

ScD, Massachusetts Institute of Technology, 1973

Interests

Diffusion in polymers

Polymer / polymer adhesion

Polymerization reaction engineering

Controlled release

Biomedical engineering

Biomedical polymers

Bioadhesion

Awards and Major Appointments

Doc. hon. causa, University of Ghent, 1999

Doc. hon. causa, University of Parma, 1999

Best Paper Award, Midwestern Meeting, American Association of Pharmaceutical Scientists, 1999

Marion B. Scott Award, Purdue University, 1999

Best Paper Award, Materials Research Society, 1998

Fellow, American Physical Society, 1998

Research Areas

Diffusion in and Dissolution of Glassy Polymers. Penetrant transport in glassy polymers may be described by two coupled processes of penetrant diffusion and macromolecular relaxation. Dissolution of glassy polymers can be considered as a combination of solvent penetration featuring Case II transport and polymer dissolution controlled by polymer disentanglement. Anomalous transport models are developed for solvent penetration which is coupled with a disentanglement model for polymer dissolution. Solvent penetration is controlled by the relaxation or deformation of polymer and the diffusional Deborah number is shown to be a major model parameter. In the disentanglement model, dissolution of polymer molecules requires that solvent concentration be greater than a critical gel concentration and that a polymer molecule be allowed a certain time to complete the disentanglement or diffusion movement from the gel state to liquid state. This time is assumed to be equivalent to the reptation time, which is a function of molecular weight, solvent

concentration and chain rigidity. A concept of disentanglement clock is introduced as the material time clock controlling the dissolution. The new model may explain many experimental observations, such as effects of type of solvent and polymer on dissolution rate and the thickness of the gel layer. Experimental studies are performed with well-characterized samples of polystyrene and poly(methyl methacrylate) in various solvents using laser interferometer and critical angle illumination microscopy. The solvent concentration profiles and dissolution rates are measured by ellipsometry. The necessary self-diffusion coefficient of the polymer is measured by pulsed gradient spin echo NMR spectroscopy. In addition, experimental studies are performed using poly(acrylic acid) and poly(vinyl alcohol) in water to study the influence of ionic conditions on dissolution.

Polymer/polymer Adhesion and Diffusion. The interdiffusion of compatible polymer / polymer pairs is studied using scanning electron microscopy, transmission electron microscopy and attenuated total reflectance, and Fourier transform infrared spectroscopy. We examine the effect of molecular weight distribution of one component on the interdiffusion process and investigate the importance of branching and hydrogen bonding. Studies are performed with polystyrene / poly(vinyl methyl ether), polystyrene / polychlorostyrene, poly(vinyl chloride) / poly(ethyl methacrylate), and poly(vinyl chloride) / poly(methcrylate) systems. The results and associated molecular analysis have applications in healing and adhesion polymers.

Multifunctional Polymerization Kinetics and Network Structure.The mathematical modeling of multifunctional polymerization / crosslinking reactions is investigated. A theoretical model for the prediction of initiator efficiency throughout the course of the polymerization is developed. Fundamental descriptions for the propagation and termination rate constants are also developed. These expressions are incorporated into the typical initiation-propagation-termination mechanism and model simulations are carried out. Kinetic gelation simulations are carried out to determine the final network structure at the specified reaction conditions. Polymerization / crosslinking of polyethylene glycol diacrylate networks is studied by exposure to UV light. Volume shrinkage on polymerization, swelling characteristics, molecular weight between crosslinks, glass transition temperature and thermal stability of the resulting networks are determined and used to analyze the crosslinked structure. By varying the length of the ethylene glycol unit between the two C=C bonds, we are studying changes in the kinetics of these polymerizations. The conversion-time profiles are obtained at different light intensities by using a calorimetric and a spectroscopic technique.

Highly Crosslinked Poly(Meth)Acrylates for Information Storage Materials. The kinetics of polymerizations of multifunctional acrylate and methacrylate monomers as well as the crosslinked structure and properties of the ensuing polymers are studied by a variety of experimental techniques. Interferometric studies are used to calculate the relaxation of the polymer during the reaction, whereas shrinkage studies are related to conversion and the structure of the reacting monomers. The mesh size of the produced networks is analyzed using swelling studies. Differential scanning calorimetry and related thermal techniques provide information about this structure and mechanical properties of these networks. The results are used to verify and improve a kinetic model

based on relaxation and to study relationships between monomer structure and applications in the information storage field.

Monte Carlo Simulations and Structural Analysis in UV Polymerizations. The project involves a detailed analysis of how the three-dimensional network structure forms in highly crosslinked polymers, coatings, resins, etc., that are produced by the polymerization of monomers in the presence of UV light. Various types of Monte Carlo simulations will be used to analyze the kinetics of polymerization and the gradual reaction of one or more double bonds in multifunctional methacrylates. This work has applications in the fields of information storage materials, biomaterials, membranes, coatings, and drug delivery systems.

Polymer Brushes and Poly(ethylene glycol) Structures: Simulations and Surface Properties. The primary goal of this research is to elucidate the effect of interdiffusion on adhesion. The selective control of the molecular weight of the polymer chains which can diffuse across an interface is essential. Thus, while good swelling behavior of the polymer base is required, the more heavily crosslinked surfaces have fewer and shorter dangling ends. The dilemma is circumvented by selectively grafting well characterized PEG chains onto crosslinked PAA surfaces. The molecular weight of the polymer chains at the surface may now be independently varied.

Self-Associating Hydrogels of Ethylene Glycol and Methacrylic Acid. The preparation, structure and properties of novel hydrogels of poly(ethylene glycol-g-methacrylic acid) copolymers are investigated. These hydrogels have been tailored so as to be sensitive to external environmental conditions, such as change of the pH, the temperature and the solvent composition. The swelling equilibrium characteristics and the diffusive properties of the gels are dependent on these external conditions and extremely sensitive to them. Such properties are of utmost importance in the development of novel separation systems. In aqueous swelling solutions at acidic pH, copolymer networks swell to a much lower extent than homopolymer networks. This behavior is attributed to complex formation between poly(ethylene glycol) and poly(methacrylic acid) segments. Nuclear Overhauser enhancement (NMR) measurements reveal that graft copolymers form complexes under a wider range of concentrations and poly(ethylene glycol) molecular weight than the two ungrafted homopolymers. This enhancement in complexation may be attributed to elimination of the unfavorable translational free energy change of complexation by covalent attachment of the complexing species.

Interpenetrating Polymer Networks. Interpenetrating polymer networks (IPN) are meshes of two different polymers which are entangled within each other; however there is no chemical bonding between them. A major advantage of IPNs is that they have superior physical as well as chemical properties over pure homopolymers. In this research, novel stimuli responsive IPNs will be synthesized from biocompatible homopolymers based upon complexation, hydrophobic interactions, and ionization equilibrium.

An ionic, complex forming IPN has been synthesized which responds to changes in temperature, pH, and solvent composition. The IPN contain two components, poly(N,N-isopropyl acrylamide) (PNIA) and

poly(methacrylic acid) (PMAA). The PNIA network is synthesized by free radical polymerization using AIBN as an initiator. This network is then swollen in a methacrylic acid solution at 25 °C and by using the same polymerization technique PMA will be synthesized. PNIA exhibits temperature dependent swelling behavior whereas PMAA exhibits pH dependent swelling behavior (Critical temperature at 35 °C). PMA and PNIA can form hydrogen bonds which can be broken by ionizing carboxylic acid groups or by changing the swelling solvent composition. Thus, an IPN consisting of two chemically independent crosslinked polymers in which proportions and properties of each polymer can be varied independently, will be formed. This network shows temperature, pH, and solvent composition dependent swelling behavior.

These networks are characterized for their swelling properties as a function of composition and polymerization reaction conditions. The chemical characterization is done by potentiometric titrations, NMR, SEM, and ATR-FTIR. These networks can be synthesized in the form of thin membranes, discs, or microparticles.

A second category of IPNS is based on amine containing polymers, viz. IPNs of poly(N,N-dimethyl aminoethyl methacrylate) (PDMAEMA) with poly(vinyl alcohol) (PVA). The synthesis is done by homopolymerizing DMAEMA by free radical polymerization and then swelling PDMAEMA in vinyl acetate monomer solution. The swollen PDMAEMA containing vinyl acetate are then irradiated with γ-rays to form an IPN of PDMAEMA with poly(vinyl acetate). This IPN can be partially hydrolyzed by the addition of dilute sulfuric acid to form poly(vinyl alcohol). At high pH (alkaline) this IPN is in a complexed state due to the hydrogen bonding between amine groups of PVA. At lower pH (acidic), the hydrogen bonded complex is broken, because of the ionization of amine groups.

Star and Dendritic Polymers for Functional Materials. Star and dendritric polymers are molecules of hyperbranched structures, often exhibiting fractal-like behavior, which start from one central core (nucleus) and consist of a large number of terminal groups with a definite geometrical growth. Polymers exhibiting this three-dimensional, hyperbranched structure are classified as star polymers and dendrimers. Star polymers are characterized by a central core which may be a slightly crosslinked polymer core from which a large number of branches of the same or different molecular structure propagate. Dendrimers and star-burst polymers, however, are a very specific class of polymers exhibiting symmetry in their three-dimensional structure. Unlike other polymers, dendritic polymers can have precisely defined architectures and surface groups, and may be prepared as non-interacting molecular ball bearings or as crosslinked networks. The size, shape, surface chemistry, flexibility, and topology can be precisely defined and controlled, and this allows for nanoscopic tailoring. The great density of surface groups may be functionally tailored for super-strong adhesives, chemical / biological molecule detection, catalysis of toxic molecules, and as interaction site with linear polymers to modify bulk / solution properties. The interior of dendritic polymers can also be functionally tailored for a variety of uses including catalysis of toxic molecules and molecular recognition, which have been demonstrated at sites covalently bonded to the interior architecture (molecular imprinting).

From a pharmaceutical and a medical point of view, these polymeric systems are particularly promising because they can serve as micro- or

nanoparticulate carriers for drug delivery systems development. In addition, because of the very large number of free arms they can be used for immobilization of drugs, cells, enzymes or antibodies, whereby a very high density of biological agent is attained in a very small volume. We are synthesizing structurally intriguing dendrimers and star polymers. These have significant potential to serve as models for the investigation of supramolecular biological interactions, as well as for the study of highly ionic polymeric systems. Of particular importance in biomedical and pharmaceutical research is their ability to act as supports for immobilization of bioactive agents. The main components of a star- burst polymer are the core or foundation site from which the diverging branches of the dendritic structure start. One or more branching arms emanate from this core site, each one incorporating a further branch point. Finally, a terminal functionality is observed for each of the branches, usually having a reactivity which allows it to further react in the dendritic structure. Dendrimers are prepared using distinct stages of monomer addition, where a separate activation process is required before each new monomer generation is added. We are investigating the polymers' structure, generation growth and functionality and are experimenting with the development of novel ionic star polymers.

pH-Sensitive Complex Hydrogels and IPNs for Drug Release. Novel carriers for controlled delivery of drugs are prepared from hydrogels that have the ability to respond to pH, ionic strength, composition of physiological solution and temperature. Such hydrogels can be used for abrupt release of drugs or proteins at constant rates. We have developed graft copolymers of poly(ethylene glycol) with poly(methacrylic acid), which can complex by hydrogen bonding. An alternative release system based on interpenetrating polymeric networks of complexing is also developed. Finally, pH-sensitive hydrogels of poly(hydroxyethyl acrylic acid) are synthesized in the presence of water at concentrations larger than the equilibrium concentrations of the corresponding gels. When these systems are loaded with drugs or proteins and swollen in constant pH solutions, they deswell (collapse) transforming the polymer system into a highly porous gel. Thus, the incorporated drugs can be released at constant rates. The release process is dependent on the pH and temperature of the solution. Experimental studies of drug release from such systems will be carried out and the overall release behavior will be modelled.

Drug Targetting to Cancerous and Other Tissues by Mucin/Polymer Interactions. The goal of this work is the development of improved polymers that can be used for wound healing or as carriers for drug targeting to specific sites of the body. The effect of crosslinking, polymer hydrophilicity, and interdiffusion on the adhesion and cohesion of hydrogel with adhesive functional groups in contact with mucin will be investigated. Hydrogels will be prepared by free radical polymerization of acrylic acid, 2-hydroxy ethyl methacrylate and ethylene glycol dimethacrylate. The surface chemistry of selected polymers will be modified by grafting poly(ethylene glycol) of varying molecular weight. The surface and bulk properties will be characterized by contact angle measurements, gas chromatography, gel permeation chromatography, differential scanning calorimetry and Fourier-transform infrared (FTIR) spectroscopy. Near-field FTIR will be used to study the interdiffusion and adhesion process in contact with mucin and identify the molecular characteristics that will provide maximum mucoadhesion.

Temperature-Sensitive Block Copolymers for Controlled Release. Environmentally sensitive hydrogels have biomedical applications in drug delivery. Temperature- and pH-sensitive hydrogels were synthesized by polymerization of poly(ethylene glycol) (PEG), methacrylic acid (MAA), and N-isopropyl acrylamide (NIPAAm), with tetraethylene glycol dimethyacrylate added as a crosslinking agent. Because of an intercomplexation mechanism between the carboxylic acid of the MAA and the ether oxygens of the PEG, these gels exhibited pH-dependent swelling. Addition of oligo-NIPAAm chains resulted in temperature sensitivity due to the existence of a lower critical solubility temperature. Equilibrium swelling studies were done to examine the network structure as a function of temperature and pH. Studies were done using dimethyl glutaric acid buffered solutions ranging in pH from 3.4 to 7.4 at temperatures ranging from 25˚C to 37˚C. Equilibrium volume swelling ratios varied by an order of magnitude from the condition of low pH and high temperature to the case of high pH and low temperature. Modulated drug release studies were performed using proxyphylline to investigate the potential for pulsatile drug delivery.

Mucoadhesive/Bioadhesive Polymers for Protein Targetting. A promising method of directed delivery of peptides and proteins is by incorporation into H-bonding controlling polymers and injection/administration in the body. We are examining the polymer/biomedical conditions of improvement of the adhesive bond between free, branched or crosslinked polymer chains and the tissue, mucus or skin. The effect of crosslinking, polymer hydrophilicity, and interdiffusion on the adhesion and cohesion of bioadhesive hydrogels in contact with mucin will be investigated. Hydrogels will be prepared by free radical polymerization of a variety of monomers. The surface chemistry of selected polymers is modified by grafting poly(ethylene glycol) of varying molecular weight (PEG-tethered structures). The surface and bulk properties are characterized by contact angle measurements, GC, GPC, DSC, TGA and FTIR spectroscopy. Near-field FTIR is used to study the interdiffusion and adhesion of gels on gels or mucin.

New Biopolymers Based on Poly(acrylic acid) and Containing Poly(ethylene glycol) Chains as Mucoadhesive Drug Delivery System. The primary goal of bioadhesive controlled drug delivery is to localize a delivery device within the body to enhance the drug absorption process in a site-specific manner. Bioadhesion is affected by the synergistic action of the biological environment, the properties of the polymeric controlled release device, and the presence of the drug itself. The delivery site and the device designed are dictated by the drug's molecular structure and its pharmacological behavior. Recent studies in our laboratory indicate that the mucoadhesive behavior of specific hydrophilic polymer structures used as carriers for drug delivery can be improved with the addition of poly(ethylene glycol) (PEG) as an adhesion promoter. PEG chains can be added to such structures by postreaction grafting leading to PEG-tethered hydrogels. An additional method is by loading PEG into an already swollen hydrogel structure. In the present work we develop, characterize and evaluate new drug delivery systems containing PEG. The fracture energy required to separate layers of hydrogel films in control with mucin is investigated to evaluate the impact of promoter chain diffusion on device/mucin adhesion and to obtain molecular information on the fracture energy in drug carrier mucoadhesion. PEG is incorporated in a hydrogel and

used as an adhesion promoter. The influence of PEG molecular weight and contact time on PEG diffusion across the hydrogel / mucin interface is investigated by using tensiometry and near-field FTIR microscopy. Fracture analysis provides details about the mechanism of muco-adhesion and conditions of improved adhesion. In our work, we concentrate also on the practical development of such PEG-tethered or PEG-promoted systems for transmucosal, buccal and nasal delivery systems.

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P. Colombo, R. Bettini and N.A. Peppas, "HPMC Matrices Containing a Soluble Drug. I. Modelling of Swelling Process and Diffusion Front Position During Swelling," *J. Controlled Release*, (in press).

N.A. Peppas, K.B. Keys, M. Torres-Lugo and A.M. Lowman, "Poly(ethylene glycol)-containing Hydrogels in Drug Delivery," *J. Controlled Release*, (in press).

R.A. Scott and N.A. Peppas, "NMR Spectroscopy and Free Volume Analysis of the Effects of Copolymer Composition on the Swelling Kinetics and Chain Dynamics of Highly Crosslinked Copolymers of Acrylic Acid and PEG-Containing Multiacrylates," *J. Polym. Sci., Polym. Phys.*, (in press).

A.M. Lowman and N.A. Peppas, "Hydrogels," in *Encyclopedia of Controlled Drug Delivery*, E. Mathiowitz, ed., Wiley, New York, NY, (in press).

B. Narasimhan, S.K. Mallapragada and N.A. Peppas, "Release Kinetics: Data Interpretation," in *Encyclopedia of Controlled Drug Delivery*, E. Mathiowitz, ed., Wiley, New York, NY, (in press).

A.M. Lowman and N.A. Peppas, "Molecular Analysis of Interpolymer Complexation in Graft Copolymer Networks," *Polymer*, in press.

A.M. Lowman, M. Morishita, T. Nagai and N.A. Peppas, "Oral Delivery of Insulin Using pH-Responsive Complexation Gels," *J. Pharm. Sci.*, (in press).

K. Podual, F.J. Doyle, III, and N.A. Peppas, "Preparation and Characterization of the Dynamic Response of Cationic Copolymer Hydrogels Containing Glucose Oxidase," *Polymer*, (in press).

K. Podual, F.J. Doyle, III, and N.A. Peppas, "Dynamic Behavior of Glucose-Oxidase-containing Microparticles of Poly(ethylene glycol)-grafted Cationic Hydrogels in an Environment of Changing pH," *Biomaterials*, (in press).

K. Podual, F.J. Doyle, III, and N.A. Peppas, "Glucose-sensitivity of Glucose Oxidase-containing Cationic Copolymer Hydrogels Having Poly(ethylene glycol) Grafts," *J. Controlled Release*, (in press).

N.A. Peppas, M.D. Little and Y. Huang, "Bioadhesive Controlled Release Systems," in *Handbook of Pharmaceutical Controlled Release Technology*, A.M. Klibanov, R. Langer, A.G. Mikos, N.A. Peppas, D.J. Trantolo, G.E. Wnek, and M.J. Yaszemski, eds., Dekker, New York, NY, (in press).

R. Scott, J.H. Ward and N.A. Peppas, "Development of Acrylate and Methacrylate Polymer Networks for Controlled Release by Photopolymerization Technology," A.M. Klibanov, R. Langer, A.G. Mikos, N.A. Peppas, D.J. Trantolo, G.E. Wnek, and M.J. Yaszemski, eds., Dekker, New York, NY, (in press).

P. Colombo, P. Santi, N.A. Peppas and R. Bettini, "Drug Release from Swelling Controlled Systems," A.M. Klibanov, R. Langer, A.G. Mikos, N.A. Peppas, D.J. Trantolo, G.E. Wnek, and M.J. Yaszemski, eds., Dekker, New York, NY, (in press).

N.A. Peppas, "Hydrogels" in "Biomaterials Science: An Introduction to Materials in Medicine," B.D. Ratner, A.S. Hoffman, F.J. Schoen and J.E. Lemons, eds., 2nd edition, Academic Press, New York, NY, in press.

N.A. Peppas, "Intelligent Hydrogels and their Biotechnological and Separation Applications," in G. Güren *Radiation Synthesis of Intelligent Hydrogels and Membranes for Separation Purposes*, IAEA, Vienna, (in press).

P. Colombo, R. Bettini, P.L. Catellani and N.A. Peppas, "Drug Volume Fraction Profile in the Gel Phase and Drug Release Kinetics in HPMC Matrices Containing a Solute Drug," *Europ. J. Pharm. Sci.* (submitted).

C.S. Brazel and N.A. Peppas, "Modelling of Drug Release from Swellable Polymers," *Europ. J. Pharm. Biopharm.*, (submitted).

C.S. Brazel and N.A. Peppas, "Recent Studies and Molecular Analysis of Drug Release from Swelling Controlled Devices," *STP Pharma*, (submitted).

A.M. Lowman and N.A. Peppas, "Solute Transport Analysis in pH-Responsive, Complexing Hydrogels of Poly(Methacrylic Acid-g-Ethylene Glycol)," *J. Biomat. Sci., Polym. Ed.*, (submitted).

Y. Huang, W. Leobandung, A. Foss and N.A. Peppas, "Molecular Aspects of Muco- and Bioadhesion: Tethered Structures and Site-Specific Surfaces," *J. Controlled Release*, (submitted).

J. Siepmann, H. Kranz, R. Bodmeier and N.A. Peppas, "HPMC Model Combining Diffusion, Swelling and Dissolution Mechanics and Predicting the Release Kinetics," *Pharm. Res.*, (submitted).

M. Ingemann, S. Frøkjaer, L. Hovgaard, N.A. Peppas and H. Brønsted, "Oral Drug Delivery of Enzymes. I. Immobilization of Phenylalanine Ammonia-lyase and Lipase in Hydrogels," *J. Controlled Release*, (submitted).

K. Nakamura, Y. Maitani, A.M. Lowman, K. Takayama, N.A. Peppas and T. Nagai, "Uptake and Release of Budesonide from Mucoadhesive, pH-Sensitive Copolymers and their Application to Nasal Delivery," *J. Controlled Release*, (submitted).

M. Torres-Lugo and N.A. Peppas, "Transmucosal Delivery Systems for Calcitonin: A Review," *Biomaterials*, (submitted).

R.S. Parker, J.H. Ward, F.J. Doyle III and N.A. Peppas, "Robust Discrete H_∞ Control of Glucose in a Diabetic Patient Using a Physiological Model," *AIChE J.* (submitted).

M. Torres-Lugo and N.A. Peppas, "Molecular Design and in vitro Studies of Novel pH-Sensitive Hydrogels for the Oral Delivery of Calcitonin," *Macromolecules*, (submitted).

J. Siepmann, H. Kranz, N.A. Peppas and R. Bodmeier, "Calculation of the Required Size and Shape of HPMC Matrices to Achieve Desired Drug Release Profiles," *Intern. J. Pharm*., (submitted).

M. Torres-Lugo and N.A. Peppas, "Molecular Design and in vitro Studies of Novel pH-Sensitive Hydrogels for the Oral Delivery of Calcitonin," *Macromolecules*, (submitted).

C.M. Hassan and N.A. Peppas, "Structure and Applications of Poly(vinyl alcohol) Hydrogels Produced by Conventional Crosslinking or by Freezing/Thawing Methods," *Adv. Polym. Sci.*, (submitted).

C.M. Hassan and N.A. Peppas, "Structure and Morphology of Freeze/Thawed PVA Hydrogels," *Macromolecules*, (submitted).

C.M. Hassan, J.E. Stewart and N.A. Peppas, "Diffusional Characteristics of Freeze/Thawed PVA Hydrogels: Applications in Controlled Release," *Europ. J. Pharm. Biopharm.*, (submitted).

C.M. Hassan, J.H. Ward and N.A. Peppas, "Modeling of Crystal Dissolution of Poly(vinyl alcohol) Gels Produced by Freezing/Thawing Processes," *Polymer*, (submitted).

C.M. Hassan and N.A. Peppas, "Cellular Freeze/Thawed PVA Hydrogels," *J. Appl. Polym. Sci.*, (submitted).

Editorial Boards

Biomaterials (1980-82); *Editor (1982-)*

Advances in Chemical Engineering; *Editor* (1999-)

Journal of Applied Polymer Science (1976-)

Polymer Gels and Networks (1993-)

Journal of Biomaterials Science, Polymer Edition (1987-)

Biomedical Materials (1985-)

Journal of Controlled Release (1983-)

Encyclopedia of Controlled Drug Delivery (1997-)

Advanced Drug Delivery Reviews (1992-)

Journal of Nanostructured Materials (1998-)

Tissue Engineering (1994-)

S.T.P. Pharma Sciences (1987-)

European Journal of Pharmaceutics and Biopharmaceutics, *U.S. Editor* (1992-94); (1992-)

Tissue Engineering Books, Academic Press (1995-)

Chemical Engineering Progress (1991-93)

Polymer News (1980-92)

Invited Lectures

"Carriers from PEG Star Polymers for Drug Delivery and Molecular Imprinting," University of Parma, Department of Pharmacy, Parma, Italy, May 19, 1998.

"Protein Delivery with Poly(ethylene glycol) Systems," University of Ferrara, Faculty of Pharmacy, Ferrera, Italy, May 21, 1998.

"Glassy / rubbery Transitions in Food Products and Importance in Flavor Release," Kellogg, Battle Creek, MI, September 23, 1998.

"Drug Delivery from PVA Networks," University of Parma, Department of Pharmacy, Parma, Italy, May 5, 1999.

Chaired Conferences/ Symposia

Chairman of Session on "Drug Delivery," 24th Annual Meeting of the Society for Biomaterials, San Diego, CA, April 1998.

Organizing Committee, Fifth European Controlled Release Meeting, Nordwijk, April 1998.

International Advisory Board, Second World Meeting on Pharmaceutics, Biopharmaceutics and Pharmaceutical Technology, Paris, May 1998.

Chairman of Session on "Biofunctional Polymers in Drug Delivery," Conference on Challenges for Drug Delivery and Pharmaceutical Technology, Tokyo, Japan, June 1998.

International Program Committee, Conference on Challenges for Drug Delivery and Pharmaceutical Technology, Tokyo, June 1998.

Organizing Committee, Ninth International Pharmaceutical Technology Symposium, Ankara, Turkey, September 1998.

Organizing Committee, US-Israel NSF Chemical Engineering Workshop, Haifa, Israel, March 1999.

Chairman of Session, US-Turkey-Israel Conference on Chemical Engineering, Haifa, Israel, March 1999.

Chairman of Symposium on "Synthesis and Characterization of Polymers for Biomaterials and Drug Delivery Carriers," ACS Meeting, Anaheim, CA, March 1999.

Meeting Presentations

"Solid-state NMR Investigation of Interpolymer Complexation in Swollen Copolymer Networks," Annual American Chemical Society Meeting, Boston, MA, August 27, 1998.

"Long-term Morphological Changes in Freeze-thawed PVA Hydrogels," Annual American Chemical Society Meeting, Boston, MA, August 27, 1998.

"Structure and Solute Size Exclusion of Poly(N-isopropylacrylamide)/ Poly(methacrylic acid) Interpenetrating Polymeric Networks," Annual American Chemical Society Meeting, Boston, MA, August 27, 1998.

"Contract Research Organizations and Their Role and Importance," Symposium on New Drug Developments in Pharmaceutical Sciences and Drug Registration, Istanbul, Turkey, September 5, 1998.

"Macromolecules as Excipients," 9th International Pharmaceutical Technology Symposium, Ankara, Turkey, September 8, 1998, Plenary Lecture.

"Excipients for Food, Cosmetic and Consumer Applications," 9th International Pharmaceutical Technology Symposium, Ankara, Turkey, September 8, 1998, Plenary Lecture.

"Poly(ethylene glycol) Star Polymer Hydrogels," Sixth Annual Chemical Engineering Graduate Student Symposium, Lexington, Kentucky, September 18, 1998.

"Kinetics and Modeling of UV Polymerizations Initiated with an Iniferter," Sixth Annual Chemical Engineering Graduate Student Symposium, Lexington, Kentucky, September 18, 1998.

"Novel pH-Sensitive Hydrogels for the Oral Delivery of Salmon Calcitonin," Sixth Annual Chemical Engineering Graduate Student Symposium, Lexington, Kentucky, September 18, 1998.

"Modelling of the Swelling Process and the Diffusion Front Position in Hydrophilic Matrices," Sixteen Meeting of ADRITELF, Pisa, Italy, October 9, 1998.

"Advances in Drug and Protein Delivery," First International Pharmaceutical Students Federation Meeting, Coimbra, Portugal, November 3, 1998), Plenary Lecture.

"A New Model Describing the Swelling and Drug Release Kinetics from HPMC Tablets," Annual American Association of Pharmaceutical Scientists Meeting, San Francisco, CA, November 13, 1998.

"Some Properties of Novel Multifunctional pH-Sensitive and Bioadhesive Polymers," Annual American Association of Pharmaceutical Scientists Meeting, San Francisco, CA, November 13, 1998.

"Biomaterials and Drug Delivery Systems," Annual AIChE Meeting, Miami Beach, FL, November 12, 1998, Plenary Lecture.

"Poly(ethylene glycol) Star Polymer Hydrogels," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"Structure and Morphology of Novel Poly(vinyl alcohol) Hydrogels Prepared by Freezing/Thawing Processes," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"Molecular Level Investigation of Interpolymer Complexation in Copolymer Gels," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"Experiments and Modelling of Ultraviolet Polymerizations," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"Uncertainty and Robustness in Diabetic Patient Blood Glucose Control," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"Preparation and Characterization of Poly(N-isopropyl acrylamide)/ Poly(methacrylic acid) Interpenetrating Polymeric Networks," Annual AIChE Meeting, Miami Beach, FL, November 14, 1998.

"pH-Sensitive Hydrogels with PEG-tethered Chains for Oral Delivery of Calcitonin," Annual MRS Meeting, Boston, MA, December 1, 1998.

"Molecular Aspects of Muco- and Bioadhesion: Tethered Structures andSite-Specific Surfaces," Ninth International Symposium on Recent Advances in Drug Delivery Systems, Salt Lake City, UT, February 22, 1999, Invited Lecture.

"Advances in Gel Science and Technology," US-Israel-Turkey NSF Meeting on Chemical Engineering, Haifa, Israel, March 10, 1999, Invited Lecture.

"The Characterization of P(PEGMA-co-PEGDMA) Gels for Use in Coating the Tract of a Transjugular Intrahepatic Porto-systemic Shunt," Annual American Chemical Society Meeting, Anaheim, CA, March 24, 1999.

"Structural and Morphological Characteristics of Carriers Based on Poly(acrylic acid)," Annual American Chemical Society Meeting, Anaheim, CA, March 24, 1999.

"pH-Dependent Swelling of Nano-sized Poly(methacrylic acid-g-ethylene glycol) Gels," Annual American Chemical Society Meeting, Anaheim, CA, March 24, 1999.

"A Thermodynamic Study of Polymer Chains Tethered on Gel Surfaces," Annual American Physical Society Meeting, Atlanta, GA, March 25, 1999.

"Poly(N-isopropyl acrylamide)/Poly(methacrylic acid) Interpenetrating Polymeric Networks in Drug Delivery," Midwestern AAPS Meeting, Chicago, IL, May 17, 1999.

"Targeted Oral Delivery of Insulin from Complexation Hydrogels," Annual Meeting of Society for Biomaterials, Providence, RI, April 30, 1999, Invited Lecture.

"Intelligent Hydrogels and their Biotechnological and Separation Applications," Meeting of International Atomic Energy Agency, Takasaki, Japan, May 18, 1999.

Doraiswami Ramkrishna

1976

Harry Creighton Peffer Distinguished Professor of Chemical Engineering

Degrees

BS, University of Bombay, 1960

PhD, University of Minnesota, 1965

Interests

Chemical reaction engineering

Dispersed phase systems

Biochemical Engineering

Applied mathematics

Awards and Major Appointments

1999 Dow-Professor Sharma Distinguished Fellow in Chemical Engineering at Bombay University.

Research Areas

Chemical Reaction Engineering. Research emphasis in reaction engineering is on orchestration of interfacial mixing and reaction to promote selectivity and conversion in heterogeneous, multiphase reactors. In collaboration with Professor Delgass, the investiga-tion of spatial patterns has shifted towards mixing catalysts in order to feature auxiliary reactions that “correct” unfavorable trends in the main reaction system. Catalyst mixing is considered from the intra pellet scale using composite pellets, to the pellet scale of mixing different pellets, and on to the reactor scale comprising layered spatial patterns of different beds with suitably varying reaction conditions. Preliminary calculations show that such patterns have the potential to vastly improve reactor operation in terms of conversion and selectivity. Analysis of the stability and sensitivity of patterns is under way with focus on the effects of pattern breaking perturbations. Applications to several commercially significant reaction systems are under investigation. Recent findings indicate the possibility that, without the aid of controlling nonlinear steady state multiplicity and dynamic stability behavior, the advantage of spatally patterned operation might be at risk.

Dispersed Phase Systems. A procedure for the inversion of dynamic particle size distributions to calculate nucleation and growth kinetics of crystallization and precipitation systems has been developed recently in our group. The advantage of this procedure lies in the identification of population balance models essential for controlling particle size in crys-tallization or precipitation processes even when models of theoretical origin are not available for nucleation and particle growth and may be of special significance to complex biological systems. With Professor Doyle of the University of Delaware, the development of algorithms for

control of particle size distributions in precipitation processes is in progress. Current work has shown that time-dependent nucleation of particle growth rates can be obtained from dynamic measurements of particle size distributions in the absence of aggregation processes. Further work is in progress towards accommodating aggregation processes.

Joint work with Professor Basaran on the deformation and break-up of droplets in random pressure fields has been undertaken towards understanding of break-up in turbulent dispersions. Boundary integral and finite element methods have been currently employed to investigate break-up of inviscid drops in non-random fields as a precursor to the foregoing problem.

Biochemical Engineering. Cybernetic modeling concepts have been applied to problems in metabolic engineering with successful applications to numerous case studies established in the literature. A collaborative proposal has been submitted to the National Science Foundation with Professors Frank Doyle at the University of Delaware, Jeff Varner at the University of Minnesota, and Alan Konopka and Cindy Nakatsu at Purdue University on metabolic engineering of ethanol production guided by cybernetic modeling.

Joint work with Professor Hu and his group at the University of Minnesota on Cybernetic Modeling of the growth of Hybridoma cells for the production of antibodies has recently shown their capacity to accommodate multiple steady state behavior in continuous bioreactors. Work is in progress towards the use of cybernetic models to guide experimentation towards maintenance of high cell density steady states promoting high productivity of antibodies.

Stochastic analysis of biological systems focusing on cell death is in progress designed towards applications to radiation of cancerous tumors, sterilization processes and so on.

Applied Mathematics. Specific applications drive research effort in applied mathematics generally from the areas of linear operator theory, stochastic processes and the solution of inverse problems.

Publications

Varner, J. and D. Ramkrishna, "Application of Cybernetic Models to Metabolic Engineering. Investigation of Storage Pathways," *Biotech. & Bioeng., 58,* 282-291, 1998.

Trinh, S. and D. Ramkrishna, "Spatiotemporal Patterns in a Catalytic Reactor," *Ind. Eng. Chem., Ind. & Eng. Chem Res.* (L. K. Doraiswamy issue) *37*, 2232-2238, 1998.

Varner, J. and D. Ramkrishna, "Metabolic Engineering from a Cybernetic Perspective-I. Theoretical Preliminaries," *Biotechnology Progress, 15*, 407-425, 1999.

Varner, J. and D. Ramkrishna, "Metabolic Engineering From A Cybernetic Perspective II. Qualitative Investigation of Nodal Architectures and Their Response to Genetic Perturbation," *Biotechnology Progress, 15*, 426-438, 1999.

Varner, J. and D. Ramkrishna, Metabolic Engineering From A Cybernetic Perspective: Aspartate Family of Amino Acids," *Metabolic Eng., 1*, 88-116, 1999.

Varner, J. and D. Ramkrishna, "Metabolic Engineering from a Cybernetic Perspective-IV. Penicillin V Biosynthetic Network," *Metabolic Eng.*, submitted.

Varner, J. and D. Ramkrishna, "Nonlinear Analysis of Cybernetic Models-I. Guidelines for Model Formulation," *J. Biotechnol.* in press, 1999.

Tobin, T. and D. Ramkrishna, "Modeling the Effect of Drop Charge on Coalescence in Turbulent Liquid-Liquid Dispersions," *Can. J. Chem. Eng.*, to appear in September 1999.

Ramkrishna, D. and R. Aris, "The Beauty of Self-Adjoint Symmetry," *Ind. Eng. Chem. Research* (Special Issue in honor of Roy Jackson), 38, 845-850 1999.

Cote, A., W. N. Delgass and D. Ramkrishna, "Investigation of Spatially Patterned Catalytic Reactors," *Chem. Eng. Sci.* (ISCRE issue), *54*, 2627-2635, 1999.

Ramkrishna, D. and J. Schell, "On Self-Similar Growth," *J. Biotechnology*, in press, 1999.

Kumar, S., T. Pirog and D. Ramkrishna, "A New Method for Estimating Creaming / Settling Velocity of Particles in Poly-Dispersed Systems," *Chem. Eng. Sci.*, in press.

Ramakrishna, R., D. Camp, A. E. Konopka and D. Ramkrishna, "Growth of Pseudomonas putida on Naphthalene and Organic Acid Mixtures," *FEMS Microbiology Letters*, submitted.

Varner, J., D. Ramkrishna and J. E. Bailey, "A Self-Optimizing Adaptive Model of Glucose Catabolism in Escherichia coli. Prediction of Network Response to Amplification of Key Glycolytic Enzymes," *Biotechnology Progress*, in press, 1999.

Varner, J. and D. Ramkrishna, "Mathematical Models of Metabolic Pathways," *Current Opinion in Biotechnology, 10*, 146-150, 1999.

Invited Lectures

Department of Chemical Engineering, University of California at Los Angeles, CA, March 6, 1998. Lecture on "Destabilization of Stored Emulsions."

Department of Chemical Engineering, The State University of New Jersey, Rutgers, Piscataway, NJ, April 16, 1998, Lecture (as part of Collaboratus VIII, Eighth Annual Merck-sponsored Distinguished Lecture Series) on "The Status of Cybernetic Modeling of Microbial Processes."

Conference on "Analysis of microbial cells at the single-cell level, "March 25-27, in Villa Olmo, at Como, Italy. Lecture on "On Corpuscular Models of Cell Populations. The Population Balance Approach."

Department of Chemical & Bioresource Engineering, Colorado State University, Fort Collins, Colorado, April 16, 1999. Lecture on "Modeling of Metabolic Regulation. The Cybernetic Approach."

Department of Civil Engineering, Purdue University, West Lafayette, Indiana, April 27, 1999. Lecture on "Modeling of Metabolic Regulation. The Cybernetic Approach."

Chemical Engineering Division, Bombay University Department of Chemical Technology, July 8-22, 1999. Gave six lectures on Population

Balances as Dow-Professor Sharma Distinguished Fellow. Also presented a popular lecture on "Modern Trends in Chemical Reaction Engineering," on August 2, 1999.

Department of Chemical Engineering, Indian Institute of Technology, Bombay, July 30, 1999. Lecture on "Destabilization of Stored Emulsions."

Meeting Presentations

Cote, A. S., W. N. Delgass and D. Ramkrishna, "Investigation of Spatially Patterned Catalytic Reactors," 15th International Symposium on Chemical Reaction Engineering, Newport Beach, California, September 13-16, 1998.

Cote, A. S., D. Ramkrishna and W. Nicholas Delgass, "Spatially Patterned Catalytic Reactors. Potential Industrial Applications," Paper No. 312b, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Ramkrishna, D., "The Packed Bed Reactor. A Modeler's Delight," Invited talk; Paper No. 302d, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Mahoney, A. W., D. Ramkrishna and F. J. Doyle, "Growth and Nucleation Rates from Dynamic Particle Size Distributions," Paper No. 230b, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Ramkrishna, D. and T. W. Pirog, "Simulation of the Creaming of Food Emulsions," Paper No. 245e, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998. (Scheduled paper could not be presented.)

Guardia, M. J., A. Europa, A. Gambhir, D. Ramkrishna and Wei-Shou Hu, "Cybernetic Model for Mammalian Cell Cultures," Paper No. 266f, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Varner, J. D., D. Ramkrishna and J. E. Bailey, "A Cybernetic Investigation of Glucose Catabolism in Escherichia Coli: Prediction of Network Response to Amplification of Key Glycolytic Enzymes," Paper No. 268k, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Varner, J. D. and D. Ramkrishna, "Steady State Multiplicity and History Dependence in Cybernetic Systems," Paper No. 251c, A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Ramkrishna, D. "Problems in Chemical Reaction Engineering. An Analyst's Perspective." Banquet talk at the Catalysis & Reaction Engineering Division Dinner," A.I.Ch.E. Annual Meeting, 1998, Miami Beach, November 15-20, 1998.

Cote, A., W. N. Delgass, and D. Ramkrishna, "Enhancement of Selective Conversion in Spatially Patterned Reactors," International Symposium on Reaction Kinetics and the Development of Catalytic Processes. Belgium, April 19-21, 1999.

Gintaras V. Reklaitis

1970

Professor and Head of the School

Degrees

BS, Illinois Institute of Technology, 1965

MS, Stanford University, 1969

PhD, Stanford University, 1969

Interests

Process systems engineering

Computer aided process operations

Batch process design, scheduling and analysis

Awards and Major Appointments

Editor-in-Chief, Computers & Chemical Engineering, Pergamon Press / Elsevier, 1994-

Member, Board of Directors, American Institute of Chemical Engineers, 1997-1999

Trustee, CACHE (Computer Aids for Chemical Engineering Education) Corp., 1979-

Advisory Board, Illinois Institute of Technology, Department of Chemical & Environmental Engineering, Illinois Institute of Technology, 1997-

Editorial Board, Computer Applications in Engineering Education, 1992-

Board of Judges, Chemical Engineering Personal Achievement Award, 1998.

Board of Judges, Kirckpatrick Chemical Engineering Achievement Award, 1999

Research Areas

Professor Reklaitis' research involves the application of computing and systems technology to support the design and operation of processing systems. A long term goal is to create a framework for and demonstrate the feasibility of fully computer integrated chemical manufacturing. Areas of recent emphasis are investigation of approaches to support batch and semicontinuous operations as well as methodology for plant- and enterprise-wide planning and optimization.

Batch process design encompasses the selection of processing recipe, operational schedules, equipment number and sizes, plant layout, and the staging of plant expansions. Batch plant design problems are challenging because they involve discrete choices, dynamics, and parameter uncertainty. Their solution requires developments in process and logistical decision modeling, combinatorial optimization techniques, combined discrete-continuous simulation methods, and probabilistic

decision tools such as Monte Carlo methods. Problems of current interest include synthesis and design for waste minimization.

Batch operational problems include the detailed scheduling of multi-purpose production facilities, taking into account technical, production, and market driven uncertainties, and the integration of scheduling decisions with enterprise-wide planning and process unit control functions. In the process setting, schedules define the assignment of equipment and other resources to manufacturing tasks, the sequencing of the execution of these tasks, and the determination of the precise timing for their execution. Areas of current interest include the investigation of techniques for developing robust schedules which give good performance in the presence of uncertainty, dynamic strategies for deciding when rescheduling is most appropriate, and the integration of scheduling models with detailed unit operational models. Applications of the latter include campaign strategies for reactive and nonreactive batch distillation operations.

Plant-wide optimization and planning research is concerned with the formulation of mathematical models and development of large scale solution strategies under which the operation of production facilities, multiple interacting plant sites, and entire supply chains can be effectively coordinated. Plant-wide real-time optimization methodology seeks to maintain the plant on an optimum operating path through a closed loop process which includes on-line plant data collection and validation, automated model parameter updating, model optimization to obtain new plant set-points, interpretation and filtering of optimization results, and implementation of updated set points on distributed control systems. Current emphasis is on hybrid systems for performing the interpretation and filtering functions and the design of RTO systems which can accommodate combined batch and continuous plant operations. The planning research is concerned with the development of models and methods for addressing problems of planning under uncertainty, including R&D planning as well as supply chain optimization applications. The technologies which are employed for these purposes include large scale linear, nonlinear, and discrete optimization methods, statistical techniques, knowledge-based methods, as well as combined discrete-continuous simulation tools.

Publications

Zentner, M.G., A. Elkamel, J.F. Pekny, and G.V. Reklaitis, "A Language for Describing Process Scheduling Problems," *Computers & Chem. Engr., 22, No.1-2.* pp. 125-145 (1998).

Wajge, R. and G.V. Reklaitis, "An Optimal Campaign Structure for Multicomponent Batch Distillation with Reversible Reaction," I&*EC Research, 37,* 1910-1916 (1998)

Pekny, J.F., and G.V. Reklaitis, "Towards the Convergence of Theory and Practice: A Technology Guide for Scheduling / Planning Methodology," in *Foundations of Computer Aided Process Operations 1998,* AIChE Symposium Series No. 320, vol.94, 91-111, (1998)

Androulakis, I.P. and G.V. Reklaitis, "Approaches to Asynchronous Decentralized Decision Making," *Computers & Chem. Engr, 23,* 339-355(1999).

Mockus, L. and G.V. Reklaitis, "Continuous Time Representation Approach to Batch and Continuous Process Scheduling - I. MINLP Formulation," *I&EC Research, 38*, 197-203 (1999)

Mockus, L. and G.V. Reklaitis, "Continuous Time Representation Approach to Batch and Continuous Process Scheduling - II. Computational Issues", *I&EC Research, 38*, 204-210 (1999)

Honkomp, S.J., L. Mockus, and G.V. Reklaitis,"A Framework for Dynamic Schedule Evaluation under Processing Uncertainty," *Computers & Chem. Engr, 23*, 595-609 (1999).

Kuriyan, K., R.G. Squires, G.V. Reklaitis, B. Morrato, R. Gutwein, and M. Evans, "The Procter and Gamble Decaffeination Project II. Implementing a Multimedia Instruction Module in Java," *Comp. Appl. Engr. Edu., 7*, 87-98 (1999)

Wajge, R.M., and G.V. Reklaitis, "RBDOPT: A General-Purpose Object-Oriented Module for Distributed Campaign Optimization of Reactive Batch Distillation," *Chem.Eng. J., 75*, 57-68(1999)

Reklaitis, G.V., and K. Bartels, "Does US Graduate Education Work for the Chemical Industry," *CHEMTECH , 29*, pp. 7-15 (1999).

Edgar, T.F., D.A. Dixon, and G.V. Reklaitis, " Vision 2020: Computational Needs of the Chemical Industry," Report of National Research Council Workshop on Impact of Advances in Computing and Communications Technologies on Chemical Science and Technology, National Academy Press, pp.74-90 (1999)

Invited Lectures

"Towards the Convergence of Theory and Practice: A Technology Guide for Scheduling / Planning Methodology," Third International Symposium on Foundations of Computer Aided Process Operations, Snowbird, Utah, July 8, 1998

"Trends, Opportunities & Models for Pan-American Collaboration in Process Systems Engineering", Pan American Workshop to Promote Collaboration in Chemical Engineering, Rio de Janeiro, August 3-5, 1998

"Systems Approach to Batch Process Engineering," Westvaco Corporation, Charleston Research Center, Charleston S.C., September 2, 1998

"Industry-Academia-Government Research Partnering: University Perspective," ChemVision 98, Houston, TX, September 23, 1998.

"Vision 2020: Computational Needs of the Chemical Industry," National Research Council, Workshop on Impact of Advances in Computing and Communications Technologies on Chemical Sciences and Technology, Washington DC, November 1-2, 1998.

"Perspectives on Planning and Scheduling Developments," Recent Developments in Computing & Systems Technology, Plenary session, AIChE Annual Meeting, Miami Beach, November 15-20, 1998.

"Vision 2020 and Process Systems Engineering," Recent Developments in Computing & Systems Technology, Plenary session, AIChE Annual Meeting, Miami Beach, November 15-20, 1998.

"Young Faculty Mentoring: Overview & Practices", Department Heads Forum, AIChE Annual Meeting, Miami Beach, November 15-20, 1998.

"Opportunities for Systems R&D for the Process Industries", Exxon Central Research, Clinton Laboratory, April 2, 1999

"Realities and Prospects of Process Scheduling Technology",McMasters Workshop on Process Scheduling, McMaster University, Hamilton, Canada, May 5, 1999

"Approaches to Uncertainty in Process Planning & Scheduling", Automation Research Center, Seoul National University, June 29, 1999

Chaired Confrences/ Symposia

Comparisons of Chemistry & ChE Graduate Programs in the Developed Countries, workshop chair, CCR Annual Meeting, Orlando, October, 1998.

Meeting Presentations

"Scheduling A Batch Serial Line under Significant Process Uncertainty," paper 243c, AIChE Annual Meeting, Miami Beach, November 1998.

"A Computational Architecture for Addressing both Combinatorial and Stochastic Aspects of Process Management Problems," paper 243f, AIChE Annual Meeting, Miami Beach, November 1998.

"Exploiting Deterministic Methods in the Treatment of Risk Analysis for Process Management Problems: An Approach for Problems Exhibiting Knapsack Structure," paper 243h, AIChE Annual Meeting, Miami Beach, November 1998.

"Developing Environmentally and Economically Sustainable Food Processing Systems," paper 245c, AIChE Annual Meeting, Miami Beach, November 1998.

Eva Sevick-Muraca

1994

Associate Professor

Degrees

BS, University of Pittsburgh, 1983

MS, University of Pittsburgh, 1985

PhD, Carnegie Mellon University, 1989

Interests

Biomedical optical imaging and spectroscopy

Optical Engineering

Inverse problems in optical engineering

Colloidal Science

Awards and Major Appointments

Elected Fellow of the American Institute of Medical and Biological Engineering, 1998.

DuPont Young Faculty Award, 1996, 1997, 1998.

National Institutes of Health Research Career Development Award, 1995-2000.

National Science Foundation Young Investigator Award, 1993 - 1998.

Beckman Laser Institute and Medical Clinic Biotechnology Resource Advisory Committee, University of California, Irvine, Beckman Institute, 1995 - 1998

Biomedical Ad hoc committee, Optical Society of America, 1994 -

Member of industrial research consortium:

National Science Foundation IUCRC for Industrial Pharmacy, Purdue University, 1995 - present.

Research Areas

The recent advances in laser diode technology and photodetection make possible the development of non-invasive sensors for biotechnology, clinical medicine, and process monitoring in the medical, chemical, and pharmaceutical industries. However, in these industries most real systems of interest multiply scatter light, making the extraction of important spectroscopic information difficult, if not impossible. One example in the biomedical domain is the propagation of near infrared light through several centimeters of tissue. Nearly everyone has observed the propagation of red light through his or her hand held near to a white light source. Near-infrared light is multiply scattered in tissues, enabling penetration into several centimeters of tissue depth, but disabling the

simple determination of important tissue optical properties which could provide biochemical information of disease status. Another example lies in the process measurement arena. While 70-80% of the chemical based industry deals with particulate or dispersed phase process streams, there is virtually no feedback control for critical parameters of particle size distribution or volume fraction since multiple light scattering prevents on-line measurement of these parameters from traditional spectroscopic analysis.

In the Photon Migration Laboratory, instrumental techniques to measure the time-dependent propagation characteristics are developed in conjunction with the integration of diffusion theory of light transport in order to determine the optical properties of highly scattering media. Four applications of photon migration are engineered in the laboratory: (1) photon migration imaging for breast cancer screening, (2) photon migration fluorescent lifetime spectroscopy in tissues and other random media, (3) particle and dispersed phase analysis of size distribution and volume fraction for on-line measurement leading to feedback control, and (4) determination of static and dynamic structures set up by particle interactions in concentrated suspensions. Laboratory research topics which span the disciplines of physics, chemistry, electrical engineering, medicine, and chemical engineering can be found in a regularly updated website: ???? http://photon.ecn.purdue.edu/~chepmi/ppml.html.

Publications

Shinde, R.R., Balgi, G.V., Richter, S.M., Banerjee, S., Reynolds, J.S., Pierce, J.E., and E.M. Sevick-Muraca, "Investigation of static structure factor in dense suspensions using multiply scattered light," *Appl. Optics, 38*, 197-204, 1999.

Banerjee, S., Shinde, R., and E.M. Sevick-Muraca. "Probing Static Structure with Multiply Scattered Light," *Journal of Colloid and Interface Science, 209*: 142-153, 1999.

Eppstein, M.J., Dougherty, D.E., Troy, T.L., and E.M. Sevick-Muraca, "Biomedical Optical tomography using dynamic parameterization and Bayesian conditioning on photon migration measurements," *Appl. Optics, 38*: 2138-2150, 1999.

Roy, R. and E.M. Sevick-Muraca, "Truncated Newton's optimization scheme for absorption and fluorescence optical tomography: Part I Theory and Formulation," *Optics Express, 4:* 353-371, 1999.

Shinde, R.R., Balgi, G.V., Richter, S.M., Banerjee, S., Reynolds, J.S., Pierce, J.E., and E.M. Sevick-Muraca, "Investigation of static structure factor in dense suspensions using multiply scattered light," *Appl. Optics, 38*, 197-204, 1999.

Eppstein, M.J., Dougherty, D.E., Troy, T.L., and E.M. Sevick-Muraca, "Biomedical Optical tomography using dynamic parameterization and Bayesian conditioning on photon migration measurements," *Appl. Optics, 38*: 2138-2150, 1999 (cover).

Roy, R. and E.M. Sevick-Muraca, "Truncated Newton's optimization scheme for absorption and fluorescence optical tomography: Part I Theory and Formulation," *Optics Express, 4*: 353-371, 1999.

Roy, R. and E.M. Sevick-Muraca, "Truncated Newton's optimization scheme for absorption and fluorescence optical tomography: Part II Reconstructions from synthetic measurements" *Optics Express, 4*: 372-382, 1999.

Roy, R. and E.M. Sevick-Muraca, "Truncated Newton's optimization scheme for absorption and fluorescence optical tomography: Part II Reconstructions from synthetic measurements" *Optics Express, 4*: 372-382, 1999.

Richter, S.M., Shinde, R.R., Balgi, G., and E.M. Sevick-Muraca, "Particle or dispersed phase characterization via measurements of photon migration in concentrated systems," World Congress on Particle Technology III, *IChemE*, pp. 14-23, 1998.

Eppstein, M.J., Dougherty, D.E., Troy, T.L., and E.M. Sevick-Muraca, "Stochastic optical tomography using beta-distributed parameters to model absorption, lifetime, and quantum efficiency," *Biomedical Imaging: Reporters, Dyes, and Instrumentation,"* D.J. Bornhop, C.H. Contag, and E.M. Sevick (eds)., *Proc. Soc. Photo-Opt. Instrum. Eng., 3600:* 000-000, 1999.

Eppstein, M.J., Dougherty, D.E., Hawrysz, D.J., and E.M. Sevick-Muraca, "Three-dimensional optical tomography," *Optical Tomography and Spectroscopy of Tissue III*, B. Chance, R.R. Alfano, and B.J. Tromberg (eds)., *Proc. Soc. Photo-Opt. Instrum. Eng., 3597*: 000-000, 1999.

Reynolds, J.S., Thompson, A.B., Troy, T.L., Mayer, R.H., Waters, D.J., and E.M. Sevick-Muraca, "Multi-pixel frequency-domain imaging of spontaneous canine breast disease using fluorescent contrast agents," *Biomedical Imaging: Reporters, Dyes, and Instrumentation,*" D.J. Bornhop, C.H. Contag, and E.M. Sevick (eds)., *Proc. Soc. Photo-Opt. Instrum. Eng., 3600*: 000-000, 1999.

Lee, J. and E.M. Sevick-Muraca, "Fluorescence-enhanced absorption and lifetime imaging," *Biomedical Imaging: Reporters, Dyes, and Instrumentation,*" D.J. Bornhop, C.H. Contag, and E.M. Sevick (eds)., *Proc. Soc. Photo-Opt. Instrum. Eng., 3600*: 000-000, 1999.

Roy, R. and E.M. Sevick-Muraca, "Imaging of absorption coefficients and lifetime in scattering media with heterogeneous fluorophore distribution using simply bound constrained minimization," *Biomedical Imaging: Reporters, Dyes, and Instrumentation,*" D.J. Bornhop, C.H. Contag, and E.M. Sevick (eds)., *Proc. Soc. Photo-Opt. Instrum. Eng., 3600*: 000-000, 1999.

Editorial Boards

Journal of Biomedical Optics, 1998-present.

mistry and Photobiology (Associate Editor), 1995 - present.

Invited Lectures

"Biomedical optical imaging using frequency-domain photon migration," IUPUI Graduate Physics Department Colloquium, Indianapolis, IN September 10, 1998.

"Biomedical optical tomography using fluorescence photon migration," Graduate Chemistry Seminar Series, University of Iowa, Iowa City, October 2, 1998.

National Institutes of Health Diagnostic Imaging and Radiology Study Panel, 1998- 2003.

Journal of Biomedical Optics, 1998-present.

Photochemistry and Photobiology (Associate Editor), 1995 - present.

National Institutes of Health Diagnostic Imaging and Radiology Study Panel, 1998- 2003.

Chaired Conferences/ Symposia

"Biomedical optical tomography using fluorescence photon migration," Graduate Chemistry Seminar Series, University of Iowa, Iowa City, October 2, 1998.

"Biomedical optical tomography using fluorescence photon migration," Departments of Chemical and Materials Engineering, University of Kentucky, Lexington, October 13, 1998.

"Characterization of dense colloid systems using photon migration," Chemical and Petroleum Engineering Graduate seminar, University of Pittsburgh, PA, October 23, 1998.

"Biomedical optical imaging using frequency-domain photon migration," Chemical and Biochemical Engineering Graduate Seminar Series, Rutgers University, New Brunswick, NJ, November 6, 1998.

"Biomedical optical tomography using fluorescence photon migration," Chemical Engineering Graduate Student seminar, Texas A&M, College Station, TX February 5, 1999.

"Biomedical optical tomography using fluorescence photon migration," Chemical Engineering Graduate Seminar, University of California at Santa Barbara, March 18, 1999.

"Biomedical optical tomography using fluorescence photon migration," Chemical Engineering Graduate Seminar, University of California at Los Angeles, March 19, 1999.

"Photon Migration," 9th International Diffuse Reflectance Conference, Council for Near Infrared Spectroscopy, Chambersburg, PA, August 10, 1998.

"Application of photon migration measurements in the pharmaceutical industry," Pfizer Research Headquarters, Groton, CT, February 9, 1999.

"Photon migration for colloidal particle sizing in concentrated suspensions," Union Carbide, Charleston, WV April 28, 1999.

Meeting Presentations

National Academy of Engineering, Fourth Annual Meeting of the Frontiers of Engineering Symposium, Chemical Engineering / Bioengineering, September 1998 (Session Organizer and Chair).

"Non-invasive Fluorescence Techniques," in 1998 Annual Meeting of the Optical Society of America, Baltimore, MD, October 1998.

"1998 Optical Society of America Annual Meeting: Sensing the world around us," Organizing Committee, Baltimore, MD October 4-9, 1998.

"Photon Migration Imaging and Diagnostics," in 1998 Annual Meeting of the Biomedical Engineering Society, Cleveland, OH, October 1998.

"Time-resolved fluorescence spectroscopy and imaging in tissues," Society of Photo-Instrumental Engineering, San Jose, January 23-29, 1999.

"Novel Biomedical Optical Spectroscopy, Imaging, and Diagnostics," CLEO / Europe EQEC Focus Meetings, Munich, Germany June 1999.

Mayer, R.H., Reynolds, J.S., and E.M. Sevick-Muraca, "Measurement of fluorescent dye optical properties in scattering media," Annual Meeting of the Biomedical Engineering Society, Case-Western University, Cleveland OH, October 11, 1998.

Troy, T.L., Reynolds, J.S., Thompson, A.B., Mayer, R.H., and E.M. Sevick-Muraca, "Photon migration imaging of fluorescent contrast agents," Annual Meeting of the Biomedical Engineering Society, Case-Western University, Cleveland OH, October 11, 1998.

Balgi, G., Shinde, R., Richter, S.M., Banerjee, S., Conder, E., Foster, M., and E.M. Sevick-Muraca, "Characterization of concentrated particulate suspensions using frequency-domain photon migration measurements," The Federation of Analytical Chemistry and Spectroscopy Societies, Austin Texas, October 11-16, 1998 (invited).

Shinde, R.R., Balgi, G.V., S. Banerjee, and E.M. Sevick-Muraca, "Reconstruction of the Static Structure of Concentrated Colloidal Dispersions Using Multiply Scattered Light," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15.,1998.

Shinde, R.S., Banerjee, S., and E.M. Sevick-Muraca, "Investigation Of Depletion Interactions In Concentrated Suspensions By Multiply Scattered Light", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15, 1998.

Balgi, G.V., Reynolds, J.S., and E.M. Sevick-Muraca, "On-line Monitoring of Changes in Size Distribution of Cell-Debris Suspension Using Frequency Domain Photon Migration," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15,1998.

Richter, S.M., Shinde, R.R., and E.M. Sevick-Muraca, "Pharmaceutical Process Monitoring With Frequency Domain Photon Migration Measurements," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15, 98.

Richter, S.M. and E.M. Sevick-Muraca, "Photon Migration as a Tool for Monitoring Emulsion Polymerization," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15,1998.

Troy, T.L., Reynolds, J.S., Mayer, R.H., and E.M. Sevick-Muraca, "Fluorescent Lifetime Spectroscopy and Imaging in Random Media," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, Nov. 11-15,1998.

Lee, J., and E.M. Sevick-Muraca, "Born reconstruction of fluorescent lifetime and quantum efficiency from simulated measurements of frequency-domain photon migration measurements in scattering media," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Thompson, A.B., Troy, T.L. , and J.S. Reynolds, "Multipixel assessment of fluorescence phase and modulation contrast: effect of uptake, lifetime, and modulation frequency for detection of fluorescent tissue volumes," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Troy, T.L., Mayer, R.H., Waters, D., and E.M. Sevick-Muraca, "Non-compressive multi-pixel frequency-domain photon migration imaging

of spontaneous canine breast disease using fluorescent contrast agents," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Roy, R. and E.M. Sevick-Muraca, "Imaging of absorption coefficients and fluorescent lifetime in scattering media," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Hawrysz, D., Reynolds, J.S., and E.M. Sevick-Muraca, "Frequency encoding of source position for multi-source reflectance imaging measurements using frequency-domain photon migration," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Troy, T.L., and E.M. Sevick-Muraca, "Reconstruction of fluorescent lifetime and quantum efficiency: influence of modulation frequency," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Troy. T.L., Reynolds, J.S., Mayer, R.S., Waters, D., Tune, K., and E.M. Sevick-Muraca, "Image contrast using to pharmacologically altered uptake of fluorescent contrast agents in a canine model of spontaneous breast tissue disease," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Eppstein, M.J., Dougherty, D.E., Troy, T.L., and E.M. Sevick-Muraca, "Stochastic optical tomography employing beta distributed parameters to model absorption, scattering, lifetime, and quantum efficiency," Society for Photo-Instrumentation Engineering, San Jose, CA January 23-29, 1999.

Balgi, G., Reynolds, J.S., Shinde, R.R., Mayer, R.H., and E.M. Sevick-Muraca, "Photon migration sensors for monitoring powder blend homogeneity in pharmaceutical mixing operations," Thirteenth I nternational Forum of Process Analytical Chemistry, San Antonio, TX, January 24-27, 1999 (invited).

Eppstein, M.J., Dougherty, D.E., Hawrysz, D.J., and E.M. Sevick-Muraca, "Three-dimensional optical tomography using APPRIZE," OSA Munich, June 1999.

Reynolds, J.S., Thompson, A., Mayer, R., Troy, T., Waters, D., Cornell, K., Synder, P., and E.M. Sevick-Muraca, "Imaging of a fluorescent contrast agent in dog model with spontaneous mammary tumors," OSA Munich, June 1999.

Richter, S.M., Shinde, R.R., Balgi, G.,, Reynolds, J.S., Mayer, R.H., and E.M. Sevick-Muraca, "Characterization of concentrated particulate suspensions using frequency-domain photon migration measurements," International Fine Particle Society, Somerset, N.J., June 9, 1999.

Shinde, R.R., Balgi, G., Banerjee, S., and E.M. Sevick-Muraca, "Probing static structure of colloidal suspensions with multiply scattered light," International Fine Particle Society, Somerset, N.J., June 9, 1999.

Shinde, R.R., Balgi, G., and E.M. Sevick-Muraca, "Photon migration sensors for monitoring blend homogeneity in pharmaceutical mixing operations," International Fine Particle Society, Somerset, N.J., June 9, 1999.

Jennifer Lynn Sinclair

1997

Associate Professor

Degrees

BS, Purdue University, 1983

MA, Princeton University, 1985

PhD, Princeton University, 1989

Interests

Gas-solid flow

LDV measurements in fluid-solid systems

CFD multiphase code development

Transport issues in microparticle drug delivery

Awards and Major Appointments

Editorial Advisory Board, Powder Technology, 1997 - Present

Teaching for Tomorrow Award, Purdue University

Trustee, CACHE Corporation, 1999 - Present

Council for Chemical Research Representative at Council for National Science Funding Presentations at Capital Hill, May 1999

Newsletter Editor, Particle Technology Forum, AIChE

National Science Foundation Review Panel, Career Awards, November 1998

National Science Foundation Review Panel, Engineering Research Centers, March 1999

Research Areas

Throughout industry, fluid-solid processes are some of the most troublesome to operate. Too little is understood about the hydrodynamics of these complex, two-phase flows to operate the systems efficiently or to reliably scale-up, design or optimize. Typically, experimental testing is performed on expensive, large-scale units for “effective” new designs or new units mimic existing units. Improved understanding and the development of reliable computational fluid dynamic (CFD) models would limit the need for expensive large-scale test facilities. Evaluation of key variables and flow parameters such as particle concentration, particle size and size distribution, inlet flow conditions and geometry, etc. can be explored without elaborate testing equipment. In addition, turn-around time for trouble shooting an existing unit could be reduced and more efficient operation could be achieved. Professor Sinclair’s research is in developing such CFD models for multiphase flows.

In order to treat flows in systems of practical size where the solids loading ratio (ratio of solids mass flux to gas mass flux) exceeds 1, particle flow models are constructed in the Eulerian framework. Professor Sinclair's research work to date has focused on the development of such models for dilute and dense-phase gas-solid flows and these models have been incorporated into the commercial CFD package Fluent, Version 4.5.

In gas-solid flows involving larger particles, stresses in the solid phase are based on an analogy between molecular motion in a gas and particulate solids. Similar to molecules in a gas, the collisions between solid particles give rise to a random particle motion associated with individual particles which is superimposed on the bulk flow. Furthermore, the intensity of this random particle motion, referred to as the pseudothermal or granular energy, affects the pressure and viscosity of the solid phase. In dilute-phase flow, only the random motion of individual particles is important; however, in dense-phase flow, the random motion of collections of particles also occurs ("particle-phase turbulence") and contributes to the total solid phase stress. The fluctuating motion of these clusters or collections of particles is described by making an analogy to eddies in a single-phase turbulent fluid.

Effect of Particle Size Distribution. Recent work focuses on the effect of PSD since it is well known in practice that PSD plays a significant role in the flow behavior of fluid-particle systems. A small concentration of fines, for example, can significantly influence the flow of coarser particles in a fluid. In order to probe PSD effects in dilute-phase flow, particle-laden jet flow studies are conducted with particle mixtures of controlled PSD. Non-intrusive, simultaneous flow measurements of the gas and particle velocity fields are made using a three-component laser Doppler velocimeter / phase Doppler particle analyzer. Complementary modeling work has also begun involving two types of bimodal particle mixtures in dilute-phase flow. In one case, a mix of larger particles and smaller particles is considered. The small particles are assumed to follow the fluid motion closely while the fluctuating motion of the larger particles is governed by particle-particle interactions. Using a simple additive description for the drag and gas turbulence modulation, the model predictions show a reduction in pressure gradient in vertical conveying lines upon the addition of fines to the coarser particles. In the second case, a bimodal mixture of larger particles is considered in which A / A, B / B and A / B-type collisions are modeled using a kinetic theory treatment applicable to bimodal mixtures. Preliminary predictions reveal a reduction in particle phase stress in the bimodal mixture as compared to a monosized particle system with the same mean particle diameter.

Optimization of Coal Particle Flow Patterns in Low NO_X Burners. Although flame aerodynamics control the efficacy of NO_x abatement by pulverized coal burner modifications, previous research has largely focused on the chemical kinetics of NO_x formation and destruction, which is now a mature field, rather than on the fluid and coal particle flow patterns. To date, predictive methods for particle flow patterns aimed at reducing NO_x have not been used successfully to develop novel improvements in burner design and operation. One critical feature distinguishing each low NO_x burner design is the method by which the pulverized coal flame is stabilized at the burner exit, since a greatly detached flame significantly raises the NO_x emitted. Another critical feature, explored in this work, is contained in the coal injector design

details, which, together with the fluid aerodynamics, influence the subsequent environment experienced by the coal particles. In this work, the following variables are experimentally investigated in a systematic manner using LDV: flame holder geometry, secondary air swirl, inlet velocities (primary and secondary), and inlet particle concentration. Experimental results are compared to model predictions using the dilute-phase Eulerian particle flow model described above within the context of the Fluent CFD framework.

CFD Modeling of Fluidized Beds: Quantitative Analysis of Various Treatments. In this work, the aim is two-fold. First, CFD predictions for bubble size and bed expansion, using a kinetic theory description for solid-phase stresses, are compared to experimental measurements. In addition, a comparative analysis using a fluidized bed test case (Hilligardt and Werther, 1986), is undertaken to evaluate the performance of the different "common" CFD models put forth by various researchers. These models differ not only in the form of the constitutive relations but also even in terms of the governing equations, resulting in much confusion in the literature.

Publications

P. Agarwal and J.L. Sinclair, "The Effect of Particle Size Distribution on the Flow Behavior of Gas-Solid Suspension," *Fluidization IX*, L.S. Fan and T. Knowlton, eds., Engineering Foundation, NY (1998) 477-485.

J.L. Sinclair, "Case Studies for CFD in Fluid-Particle Flows," *Chemical Engineering Education* (1998*) 32,* 102-108.

J.L. Sinclair and H. Massah, "CFD in Particle Laden Flows," Numerical Methods for Multiphase Flows, *ASME-FED* (1998) *3,* 7-14.

J.L. Sinclair and T. Mallo, "Describing Particle-Turbulence Interaction in a Two-Fluid Framework," Experimental Needs for CFD Code Validation, *ASME-FED* (1998) *4,* 7-14.

T. Mallo, C. Hrenya, S. Miller, and J.L. Sinclair, "Comparison of Low Reynolds k-e Models for Predicting Heat Transfer Rates for Pipe Flow," *Int. J. of Heat and Mass Transfer* (1998), *41,* 1543-1547.

C. Yurteri, H. Massah and J.L. Sinclair, "Investigating the Effect of Gas and Particle Phase Turbulence on Developing Riser Flow using CFD," *Proceedings of the Topical Conference on Advanced Particle Technologies,* 1998 Annual AIChE Meeting, Miami Beach, Florida (1998) 483-488.

S. Vinay, M. Jhon, D. Finseth and J.L. Sinclair, "Particle Interactions in Electrostatic Separators," *Proceedings of the Topical Conference on Advanced Particle Technologies,* 1998 Annual AIChE Meeting, Miami Beach, Florida (1998) 56-62.

M. Schabel, T. Peterson, J. Sinclair and D. Lynch, "Characterization of Trapped Particles in RF Plasmas using LDV," *J. Appl. Phys.* (1999) accepted.

J. Sinclair, "A Course Project in Particle Technology, *Chemical Engineering Education* (1999) submitted.

G. Sinclair, K. Laskowitz, and J. Sinclair, "Gender Differences in Teams," *Journal of Engineering Technology* (1999) submitted.

B. Van Wachem, J. Schouten, R. Krishna, C. van den Bleek and J. Sinclair, "CFD Modeling for Gas-Solid Flows: Qualitative and Quantitative

Comparative Analysis of the Various Treatments," Numerical Methods for Multiphase Flows, *ASME-FED* (1999), submitted.

Chaired conferences/ Symposia

"Fluid-Particle Interactions" Session, 1998 Annual AIChE Meeting, Miami Beach, FL, November 1998

Emerging Technologies Workshop, "CFD for Multiphase Flow", 1998 Annual AIChE Meeting, Miami Beach, FL, November 1998

AIChE National Fluid Mechanics Programming Committee, 1996 - present

Invited Lectures

International Fine Particle Research Institute, Annual Meeting, "Dilute and Dense Phase Gas-Solid Flows," Brighton, England, June 1998.

Tioxide Ltd, "CFD for Multiphase Flow," Teeside, UK, June 1998.

Cray Research, "CFD for Multiphase Flow," Minneapolis, MN, July 1998.

Millenium Inorganic Chemicals, "Modeling Gas-Solid Flows with Particle-Particle Interactions," Baltimore, MD, October 1998.

University of Cincinnati, "Dilute and Dense-Phase Gas-Solid Flow," Department of Chemical Engineering, Cincinnati, OH, October 1998

DOE-Office of Industrial Technologies, "CFD for Multiphase Flow," Washington, DC, February 1999.

Purdue University, "Dilute and Dense-Phase Gas-Solid Flow," Agricultural and Biological Engineering, West Lafayette, IN, March 1999.

Reaction Engineering International, "CFD for Multiphase Flow," Salt Lake City, UT, May 1999.

Meeting Presentations

"Investigating the Effect of Gas and Particle Phase Turbulence on Developing Riser Flow using CFD," 1998 Annual AIChE Meeting, Miami Beach, FL, November 1998.

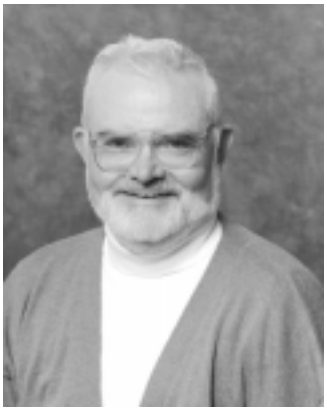
"Role of Particle Interactions in Electrostatic Separators," 1998 Annual AIChE Meeting, Miami Beach, FL, November 1998

"LDV Measurements of Particle Velocity Fluctuations in Confined Jet Flows," Fluid-Particle Interactions Conference, Engineering Foundation, Santa Fe, NM, May 1999.

Robert G. Squires

1962

Professor



Degrees BS, Rensselaer Polytechnic Institute, 1957
MS, University of Michigan, 1958
PhD, University of Michigan, 1963

Interests Educational applications of computer simulation

George T. Tsao

1974

Professor and Director of the Laboratory of Renewable Resources Engineering (LORRE)

Degrees

BS, National Taiwan University, 1953

MS, University of Florida, 1956

PhD, University of Michigan, 1960

Interests

Water purification and conservation

Biochemical Engineering

Renewable Resource Engineering

Publications

Zheng, Yizhou, H. M. Lin, and G. T. Tsao, "Pretreatment for Cellulose Hydrolysis by Carbon Dioxide Explosion," *Biotechnol. Prog. 14*, 890-896 (1998).

Tsao, G. T., N. J. Cao, J. X. Du and C. S. Gong, "Production of Multi-functional Organic Acids from Renewable Resources," *Advances Biochem Eng./Biotechnol*. (in press).

Tsao, G. T. , N. J. Cao, and C. S. Gong, "Repeated Solid Phase Fermentation and Extraction for Enzyme Production," *Applied Biochem. Biotechnol* (in press).

Gong, C. S., N. J. Cao, J. X. Du, and G. T. Tsao, "Ethanol Production from Renewable Resources." *Advance Biochem. Eng./Biotechnol*. (in press)

Gong, C. S., J. X. Du, N. J. Cao and G. T. Tsao, "Co-Production Ethanol and Glycerol by Yeasts," *Applied Biochem. Biotechnol.* (in press).

Xia, L., C. S. Gong, and G. T. Tsao, "Solid State Fermentation with Aspergillus niger for Cellobiase Production," *Applied Biochem. Biotech.* (in press).

Tsao, G, T., J. X. Du, N. J. Cao, and C. S. Gong, "Production of High Concentration of Citric Acid bt Aspergillus niger in A Bubble Column," *Applied Biochem. Biotechnol.* (in press).

Zhou, Y., J. Du, and G. T. Tsao, "Investigation of Mycelial Pellet Formation by Rhizopus oryzae ATCC 20344," *Applied Biocehm Biotechnol.* (in press).

Krishnan, M. S., Nancy Ho, and G. T. Tsao, "Fermentation Kinetics of Ethanol Production from Glucose and Xylose by Recombinanat Saccharomyces 1400(pLNH 33)," *Applied Biochem. Biotechnol. 77-79*, 373 (1999).

Zhou, Y., J. M. Dominguez, N. Cao, J. Du, and G. T. Tsao, "Optimization of L-Lactic Acid Production from Glucose by Rhizopus oryzae ATCC 52311," *Applied Biochem. Biotechnol. 77-79*, 401 (1999).

Wang, F. S., C. H. Jing, and G. T. Tsao, "Fuzzy Decision Making Problems of Fuel Ethanol Production Using a Genetically Engineered Yeast," *Ind. Eng. Chem. Res. 37*, 3434-3443 (1998).

Gong, C. S., N. J. Cao, and G. T. Tsao, "Organic Compounds, Cellulose Conversion," a review, in *Encyclopedia of Bioprocess Technology: Fermentation, Biocatalysis & Bioseparation.* 1895-1905, (1999).

Tsao, G. T., N. J. Cao, and C. S. Gong, "Hemicellulose Conversion," a review, in *Encyclopedia of Bioprocess Technology: Fermentation, Biocatalysis, & Bioseparation*. 1391-1400 (1999).

Venkat Venkatasubramanian

1988

Professor

Degrees

BTech, Chemical Engineering, Univ. of Madras, India, 1977

MS, Physics, Vanderbilt University, 1979

PhD, Chemical Engineering, Cornell University, 1984

Interests

Process fault diagnosis and supervisory control

Process hazards analysis

Computer-aided molecular design and product formulation

Synthesis of operating procedures for batch process plants

Behavior of complex adaptive systems

Intelligent systems, neural networks, and genetic algorithms

Major Appointments

Visiting Fellow, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, U.K., 1997-99.

Member of the New Technology Task Force, American Institute of Chemical Engineers, 1996-99

Trustee, CACHE Corporation, 1996-99

Research Areas

The following describes current research projects in the Laboratory for Intelligent Process Systems (LIPS) in the School of Chemical Engineering. More details and updates on the various projects and personnel in LIPS can be accessed through the World Wide Web location http://lips.ecn.purdue.edu/~lips/.

Abnormal Situation Management. Abnormal situations arise in chemical plants when plants deviate from normal operational modes. Abnormal Situation Management (ASM) deals with the timely detection, diagnosis and correction of abnormal conditions. Early diagnosis of process faults while the plant is still operating in a controllable region can help avoid event progression and reduce the amount of productivity loss during an abnormal event. The problem of fault diagnosis and subsequent control is made much more difficult by the scale and complexity of modern plants. Since the chemical process industries lose an estimated $20 billion every year, they have rated ASM as their number one problem that needs to solved. Recognizing the importance of ASM, the Abnormal Situation Management (ASM) Consortium, a technology-development partnership of leading oil companies and software vendors led by

Honeywell, to develop an intelligent system environment for operator support, called Abnormal Event Guidance and Information System (AEGIS) was formed in 1995.

As it turns out, there is no single diagnostic approach that can successfully address all the complexities of industrial-scale diagnostic problems. Hence we have designed a hybrid, blackboard-based diagnostic environment called DKit, wherein weaknesses of one technique are compensated by the strengths of the other resulting in collective problem solving. The current version of DKit, implemented in G2, combines causal model-based diagnosis with statistical techniques and qualitative trend analysis (QTA) and has been tested extensively on the Model IV FCCU.

The ASM consortium has been testing the QTA methodology developed in our laboratory at an Exxon plant for the past year and a half. There are a number of challenges with this real-life, large-scale implementation: the need to process real-time data every minute from nearly 500 sensors, the need to distinguish between operational and abnormal events, the constant shifting of the normal operating regime, incomplete operator logs and annotations, etc. The system, however, has performed very well under these conditions. Currently the consortium is planning on applying the QTA technique to other plant sites. Honeywell formally obtained an exclusive license for the QTA technology from Purdue in June 1999 in order to develop commercial products using QTA.

Computer Aided Molecular Design. The systematic identification of novel molecular products and innovative materials with optimal values of thermophysical, mechanical and/or biological properties is a key technical challenge with obvious commercial applications. The design of new molecules consists of two phases: (i) the forward problem, which involves modeling interactions between basic structural units toward property prediction and (ii) the inverse problem, which involves discovery of viable structures that are predicted to possess desired performance characteristics. In many industrial design situations where data is less and noisy, the fundamental understanding of the system is limited and time and resource constraints are stringent, a synergistic approach of first principle chemistry/physics modeling and statistical techniques like Neural Networks seems promising for the forward problem. The inverse problem is addressed using ideas from evolutionary algorithms. It has been demonstrated that genetic algorithms (GAs) are very effective in locating globally optimal solutions for a wide variety of problems including molecular design. A distinct advantage of GA is that it makes no assumption on the nature of the forward problem.

Fuel-additives are an important component of the commercial gasoline package. The primary function of a fuel-additive is, to prevent the high-boiling components in gasoline, from forming deposits on the surfaces of the intake-valve of the internal combustion engine. The formation of the intake-valve deposit (IVD) causes cold-start and emission problems in the automobile over a period of time. These deposits are strictly regulated by the EPA for all grades of commercial gasoline. Fuel-additives are designed to scavenge the deposit forming precursors in the high-boiling fractions of the fuel and hence prevent or minimize deposit formation on the intake-valve. The design of fuel-additives becomes a lengthy and expensive procedure given the high-costs of the engine tests (about $8000 a test) that measure performance. The modeling of fuel-additive performance is a difficult one because of complexities

in the different phenomena involved. Different factors ranging from engine operating conditions to flow properties of the fuel are hypothesized to play a role in intake-valve deposit formation. This precludes a purely fundamental modeling approach. On the other hand, the limited and noisy experimental data makes a completely statistical approach difficult if not fruitless. A hybrid first-principles and statistical approach has been developed to address this complex problem. In this effort the underlying phenomena responsible for imparting thermal stability to the additive in the fuel is modeled and a functional descriptor determined directly from the structure of the additive and the fuel characteristics. The descriptors are then correlated to the experimental IVD data from engine tests through a neural-network model. Due to the use of phenomena-rich functional descriptors, the neural-network was able to provide a parsimonious and accurate model. This forward model was used in tandem with an evolutionary algorithm employing specialized representation and operators to discover novel and optimal fuel-additive structures that minimize intake-valve deposits.

Similar concepts are used in the formulation and design of rubber, which has been a major engineering material for over hundred years. Rubber's elasticity and resilience have resulted in applications in load carrying structural bearings, springs, seals, shock absorbing bushes, couplings and tires. However unlike metal which require relatively few properties to characterize their behavior, the behavior of rubber is complex. It is non-linear in terms of both material and geometric behavior. Its mechanical behavior is further complicated by much greater sensitivity to the effects of temperature, processing conditions, loading rate and amount of strain. This has meant that for much of the history of rubber as an engineering material, its applications have been developed largely by trial and error, rather than by a fundamental understanding. Therefore the current endeavors are focussed towards developing an intelligent system which will help the formulator come up with rubber formulations that meets the desired property values as specified by the formulator which could include Scorch time, 95% cure, 100% modulus, 300% modulus and Compression Set. We anticipate that the intelligent system will be a combination of first-principles based chemistry / physics model working in a synergistic fashion with artificial intelligence models like neural networks to predict the long term performance of engineering materials.

Batch Process Development — Operating Procedure Synthesis and Process Hazards Analysis. Several activities need to be performed prior to start of production in a batch processing facility. These include operating procedure synthesis (OPS), process hazards analysis (PHA), scheduling, and generation of batch control code. OPS generates the instructions an operator needs to manage a batch process. PHA determines hazards that could occur when performing this sequence of operations and develops safety recommendations based on this analysis. Scheduling optimally allocates resources and equipment for each operation in the sequence generated by OPS and control code generation implements the sequence in a procedural control system. All these involve considerable amount of time, effort and expertise from plant engineers. Automation of these tasks is therefore desirable and important. Significant progress has been made recently in techniques and software for automating each of these individual functions.

Integration of these software tools is the next step in this direction and will lead to use of consistent process and plant information across these activities thereby eliminating redundancy. At our laboratory we have addressed the issues involved in integrating two software tools iTOPS, an Intelligent Tool for Operating Procedure Synthesis and BatchHAZOPExpert geared towards OPS and PHA respectively. To integrate iTOPS and BHE into one unified system it is necessary to pursue two goals - resolve the different "views" that underpin the models in the individual techniques and provide user interface and database support to allow for flow of information across the two applications.

The basic framework for iTOPS uses grafchart-based concepts to model the process at the four levels identified in S88. It uses a hierarchical planning technique to synthesize the operating procedures. iTOPS starts with information about the process materials, equipment, and chemistry to synthesize the procedure, unit procedures, operations, and phases for the process. The operating procedures are then generated from the phases. The basic framework for BHE uses a two-layered Petrinet (PN) based model of the process. The top layer called the recipe Petrinet includes information at the level of unit procedures and the bottom level referred to as the task Petrinet consists of information at the level of operations. In addition to the two-layered process model BHE also requires information about the process materials,equipment, and chemistry. Using this process information coupled with a signed digraph (SDG) based causal model BHE performs hazard and operability (HAZOP) analysis. In the integrated system the user inputs the information about the process -the materials, the chemistry, and the equipment through a top-level interface. iTOPS then uses this information to synthesize the top three process levels - procedure, unit procedures, and operations. The unit procedures and operations are then converted through an interface from a grafchart-based to a petri net-based representation to be used in BHE. BHE then performs HAZOP using this information. Meanwhile, iTOPS synthesizes the phases. After BHE has performed HAZOP analysis and iTOPS has synthesized the phases the details as to which processing steps are safety critical are transferred from BHE through the interface back to iTOPS. Safety instructions corresponding to these are then created and incorporated along with the basic instructions generated by iTOPS in the final batch record document provided to the operator.

The integrated system has been implemented in Gensym's object-oriented expert system environment, G2. The integrated system is being tested on Searle's pharmaceutical case studies and the results demonstrate the synergism achieved by integrating these techniques. In future it is proposed to extend the capabilities of the integrated system to perform other functions such as scheduling and generation of batch control code.

Publications

R. Srinivasan, V. Venkatasubramanian, "Automating HAZOP analysis of batch chemical plants: Part I. The knowledge representation framework," *Computers & Chemical Engineering 22 (9)* (1998), pp. 1345-1355.

R. Srinivasan, V. Venkatasubramanian, "Automating HAZOP analysis of batch chemical plants: Part II. Algorithms and application," *Computers & Chemical Engineering 22 (9)* (1998), pp. 1357-1370.

S. Viswanathan, C. Johnsson, R. Srinivasan, V. Venkatasubramanian, K.E. Arzen, "Automating operating procedure synthesis for batch processes: Part I. Knowledge representation and planning framework," *Computers & Chemical Engineering 22 (11)* (1998), pp. 1673-1685.

S. Viswanathan, C. Johnsson, R. Srinivasan, V. Venkatasubramanian, K.E. Arzen, "Automating operating procedure synthesis for batch processes: Part II. Implementation and application," *Computers & Chemical Engineering 22 (11)* (1998), pp. 1687-1698.

H.Vedam and V.Venkatasubramanian "PCA-SDG based Process Monitoring and Fault Diagnosis," *Control Engineering Practice 7: (7)* 903-917, Jul 1999.

S. Viswanathan, J. Zhao, V. Venkatasubramanian, L. Mockus, J.M. Vinson, A. Noren, Prabir. K. Basu, "Integrating Operating Procedure Synthesis and Hazards Analysis Automation Tools for Batch Processes," Proceedings of the European Symposium for Computer Aided Process Engineering 9, Budapest, Hungary, May 1999.

A. Sundaram, P. Ghosh, V. Venkatasubramanian, "GENESYS: A Framework for Designer Guided Evolutionary Search for high performance products," Proceedings of the European Symposium for Computer Aided Process Engineering 9, Budapest, Hungary, May 1999.

H. Vedam, S. Dash, and V. Venkatasubramanian, "OP-AIDE: An Intelligent System for Operator Support in Complex Process Plants," Proceedings of the European Symposium for Computer Aided Process Engineering 9, Budapest, Hungary, May 1999.

A. Sundaram, P. Ghosh, V. Venkatasubramanian, "Design of Fuel Additives Using Hybrid Neural Nets and Evolutionary Algorithms," Proceedings of the Foundations of Computer Aided Process Design Conference, Colorado, July 1999

Invited Lectures

"Intelligent Systems for Abnormal Situation Management," Department of Chemical Engineering, University of Newcastle upon Tyne, Newcastle, U.K., Oct 1998.

"Recent Progress in Real-time Fault Diagnosis of Complex Chemical Plants," Indian Institute of Technology, Mumbai, India, Dec 1998.

"Model Engineering of the Qualitative Trend Analysis Approach for Process Diagnosis," Honeywell Technology Center, Minneapolis, MN, Feb 1999.

"Intelligent Systems for Online and Offline Process Safety: Challenges and Opportunities," Department of Chemical Engineering, Carnegie Mellon, Pittsburgh, PA, April 1999.

Meeting Presentations

V. Venkatasubramanian, S. Viswanathan, L. Mockus, Jonanthan. M. Vinson, Prabir. K. Basu, "Automated Batch Record Generation for Pharmaceutical Plants," AIChE Annual Meeting, Miami Beach, FL, Nov 1998

S. Viswanathan, R.Srinivasan, J. Zhao, V. Venkatasubramanian, Jonanthan. M. Vinson, A. Noren, Prabir. K. Basu, "Automated Process Hazards Analysis of Batch Chemical Plants," AIChE Annual Meeting, Miami Beach, FL, Nov 1998

H. Vedam and V. Venkatasubramanian “A B-Splines-based adaptive trend analysis algorithm for process monitoring” AIChE Annual Meeting, Miami, FL, Nov 1998.

H. Vedam and V. Venkatasubramanian “Automated Fault diagnosis using principal component analysis and signed digraphs” AIChE Annual Meeting, Miami Beach,FL, Nov 1998.

Nien-Hwa Linda Wang

1980

Professor

Degrees

BS, National Taiwan University, 1971

MS, University of Wyoming, 1973

PhD, University of Minnesota, 1978

Biochemical Separation and Purification

Interests

Environmental Applications of Separation Techniques

Adsorption of Chemicals and Biochemicals

Mass Transfer in Chemical and Biological Systems

Multicomponent Batch Chromatography and Simulated Moving Bed Chromatography

Research Areas

Multicomponent Adsorption and Chromatography. Dr. Wang's group has made significant contributions in the area of multicomponent adsorption and chromatography. Their fundamental studies on the intrinsic adsorption kinetics of macromolecules show that the well known Langmuir kinetics equation, which does not take into account steric hindrance at high surface coverage, can not explain breakthrough curves of proteins at high loading. Computer simulations that consider steric hindrance are used to develop modified kinetic equations to fully explain the observed adsorption kinetics that are much slower than predicted by the Langmuir kinetics (Jin et al. 1993).

This study has also been extended to mixtures of solutes of different sizes (Talbot et al. 1993). The theoretical analysis predicts that multicomponent mixtures of molecules of different sizes show many unusual chromatographic phenomena because surface accessibility to a given solute is highly sensitive to the sizes of competing solutes, surface coverage, and local composition. Their recent studies on asymmetric solutes show that the competition between energetic factors and steric hindrance factors leads to a gradual transition from side-on orientation at low coverage to end-on orientation at high coverage. As a result, the adsorption equilibria of asymmetric solutes can not be correlated by the well known Langmuir isotherm equation. They have proposed a new isotherm equation for asymmetric solutes (Jin et al. 1999). Since most solutes are asymmetric, this correlation should be of wide interest to the adsorption field.

Their studies on mass action effects and parallel pore and surface diffusion in multicomponent chromatography are also important contributions.

Exchange of multivalent ions with monovalent ions cannot be described by the equilibrium form of the Langmuir equation. Mass action effects are demonstrated using examples in which highly concentrated solutions of monovalent ions act as effective displacers to concentrate and displace multivalent ions. The model predictions agree closely with the breakthrough curves and displacement effluent histories for multicomponent ion exchange of two, three, and five component systems (Ernest et al. 1997). A related study shows that at low concentrations, both pore diffusion and surface diffusion give symmetric breakthrough curves, which can be explained by either a pore diffusion model, a surface diffusion model, or a linear driving force (lumped) model. At high loading, however, surface diffusion gives highly asymmetric breakthrough curves, which can not be explained by pore diffusion or the lumped model. A parallel pore and surface diffusion model has been developed for multicomponent adsorption in fixed beds and expanded beds; the model gives close predictions of multicomponent breakthrough curves of organics, amino acids, and ions (Ma et al. 1996; Koh et al. 1997; Ernest et al. 1997

VErsatile Reaction SEparation (VERSE) - A Dynamic Simulation Package for Batch and Simulated Moving Bed (SMB) Chromatography. VERSE simulation is based on a detailed rate model, which takes into account (1). competitive adsorption (or ion exchange) in a multicomponet mixture, (2). detailed mass transfer mechanisms (including extracolumn dispersion, intracolumn dispersion, film mass transfer, pore diffusion, and surface diffusion), (3). slow intrinsic adsorption or desorption (compared to convection or mass transfer rates), and (4). reactions among solutes in the solution phase or among adsorbed solutes. Different modes of chromatography or adsorption processes can be simulated, including (1). frontal chromatography (saturation), (2). isocratic or gradient elution chromatography, (3). displacement chromatography, or (4). any cyclic processes involving multiple step changes in inlet feed composition, temperature, pH, ionic strength, or flow rate.

Recently, VERSE has been expanded to consider more than just the traditional single column operations. This expansion is mainly in response to the growing interest in continuous chromatography / adsorption processes. The latest features are recycle chromatography, carousel processes, and simulated moving bed processes. VERSE has been validated with many sets of batch and continuous chromatography / adsorption data for many different feed mixtures, including ions, sugars, acids, amino acids, peptides, and proteins. A list of publications related to VERSE is available in a web-based manual, which is updated from time to time. VERSE is written in FORTRAN 90 and is available on various platforms. Most widely used are Windows 95 or 98. A comprehensive on-line manual is available and it provides users with a list of available choices of isotherm functions, intrinsic kinetic rate equations, and correlations for axial dispersion coefficient and film mass transfer coefficient. Dynamic memory allocation is used in the program to perform the simulations efficiently. A minimum of 64 MB of memory (RAM) is recommended for running simulations of multicomponent systems with sharp fronts for single column operations. Carousel and SMB simulations usually require more than 64 MB RAM. Actual memory required will vary with the complexity and the acccuracy required for a specific system.

VERSE simulations can be compared with experimental data to gain fundamental understanding of complex dynamic chromatography phe-

nomena. The simulations can also provide significant cost savings in process design and development by substantially reducing the number of experiments that are normally required to study the effects of all possible operating parameters in a separation. In many applications, a pilot scale chromatography test can cost $100,000 or more. It is not practical to search for optimal designs by experimental trials. If the isotherm and mass transfer pasameters are validated with pilot scale data, VERSE simulations can be used to find the optimal design according to a given objective function. VERSE can be licensed from the Purdue Research Foundation. Several chemical and pharmaceutical companies in the US and Europe are currently using VERSE for research, process design, and process optimization.

Ion Exchange Processes for Removing Cesium from Nuclear Waste Solutions: Over the last fifty years, more than 100 million gallons of radioactive wastes generated mostly from the production of nuclear weapons have been stored in over 300 underground single-shell or double-shell tanks at Hanford, Savannah River, Oak Ridge, and other DOE facilities. It is estimated that about half of the single shell tanks are leaking, posing serious environmental threats to many states.

Efficient separation technologies are needed to treat the wastes and to allow safe long-term storage of the separated wastes. Remediation of the tank waste is estimated to cost over 100 billion dollars. This is considered by many experts one of the greatest technical and financial challenges facing the U.S. today. Major contributors to the radioactivity in the wastes are cesium and strontium. The removal of cesium, from the supernatants is an important early step in the waste treatment process. Dr. Wang's group has been collaborating with researchers from Westinghouse and Oak Ridge National Laboratories in developing an ion exchange process for the remediation. The challenge is to develop highly selective and efficient continuous processes for removing low (1-0.001mM) concentrations of radioactive Cs+ ions from concentrated aqueous solutions (1-14 M) of sodium hydroxide, sodium nitrite, and other electrolytes. They have also developed detailed dynamic models of fixed-bed ion exchange, accounting for competitive mass action ion exchange equilibria and mass transfer effects. Detailed process simulations are used to explore innovative designs of carousel processes (Ernest et al. 1997, Hritzko et al. 1998). A case study of a pilot carousel unit shows that full utilization of cesium capacity and maximum throughput can be achieved in an optimal carousel design. Reducing sorbent particle size from 400 to 290 microns, for example, increases throughput by 40% (Ernest et al. 1997). Their analysis shows that intraparticle diffusion controls wave spreading in low pressure ion exchange systems, and dimensionless mass transfer zone length is a simple linear function of particle Peclet number. To establish the linear constant of this correlation, only a few breakthrough experiments are needed for a given waste. Once the constant is found, the mass transfer zone length at a given linear velocity can be easily calculated. A robust three-segment carousel ion exchange process can be designed based on the mass transfer zone length. Dynamic simulations can be used to check switching time, transient period (time to reach steady state), column utilization, and effluent concentrations (Hritzko et al. 1999). This strategy can significantly reduce the number of expensive and time-consuming experiments in process development. Their designs are being tested experimentally for large scale waste processing.

Removal and Recovery of Organics from Water and Waste Waters. Contamination of water supplies by synthetic organics, pesticides, herbicides, and other industrial chemicals is a widespread problem in the U.S. and many other countries. Many of the chemicals are known to be carcinogenic and must be removed to safeguard drinking water supplies and the environment. Among many treatment techniques, adsorption using activated carbon beds has been the best available technology for removing dissolved organics from a dilute (ppm level) solution. Because of high selectivity, activated carbon beds can achieve virtually complete removal of many organics. This technique, however, is quite expensive. Cost of treatment ranges from $0.1 to $19.00 per 1000 gal. This high cost is due to (1) process inefficiency as a result of low throughput and low capacity utilization, (2) high capital and labor costs due to the nature of batch operation in conventional technologies, (3) sorbent attrition and incomplete, costly regeneration, and (4) loss of the organics during sorbent regeneration. Dr. Wang's group has developed a novel continuous separation process to recover amino acid derivatives and sodium chloride from a process stream containing 3.6 M sodium chloride and 40 mM of the amino acids. Thermal regeneration, instead of chemical regeneration, was developed for the continuous process. Experimental and theoretical results indicate that this continuous process is a promising solution to an important industrial problem. High purity (>95%) amino acids can be recovered at high yield (>90%). The cost of separation and recovery is estimated to be about $0.01 per gallon. They are collaborating with an industrial sponsor to explore the potential of this technology for commercial applications.

Isolation and Purification of Taxol from Plant Tissue Culture Broth and Needle Extract. Taxol, a promising anti-cancer agent, was first found in extracts from the bark of the Pacific yew tree. Because of increasing demand for taxol and limited availability of the bark, many studies have been devoted to finding alternative sources. Plant tissue culture and Taxus natural plant tissues are among the most promising alternatives. Dr. Wang and her students have developed a low pressure liquid chromatography process for the separation of taxol directly from plant tissue culture broth (Wu et al. 1996). In addition, a separation process which consists of extraction, concentration, low pressure liquid chromatography, and preparative HPLC has also been developed for the isolation and purification of taxol from Taxus needles. Their current processes can achieve high recovery (90%) and high purity (~95%). Ongoing research aims to apply simulated moving bed chromatography to improve the purity level and to further reduce the recovery and purification cost (Wu, et al. J. of Chromatography, 1999).

Simulated Moving Bed Chromatography for Biochemical Purification. In simulated moving bed chromatography, a series of columns containing a specific adsorbent are connected to form a circuit, which is divided into four zones by two inlet (feed and desorbent) and two outlet (product and by-product) ports. The four ports are periodically moved along the fluid flow direction to allow the feed to enter the region where the solute bands overlap and the products to be drawn from the regions where the bands are separated. The periodic port movement ensures high product purity and high yield in this process. It also simulates periodic counter current movement of the sorbent with respect to the ports, resulting in high sorbent utilization and high mass transfer rates. Since a major portion of the unseparated mixtures is automatically

recycled within the circuit, SMB has much higher yield and lower desorbent consumption than corresponding batch chromatography processes.

SMB, however, has not been widely used for large-scale biochemical purifications for the following reasons: (1) The SMB design is difficult, because it involves specifying a minimum of ten parameters (column diameter, four zone lengths, four flow rates, and an average port movement velocity). (2) Existing SMB's are designed for binary splits. Multicomponent separation in SMB is not yet well understood from the literature.

Dr. Wang's group has recently developed a standing wave analysis for continuous moving bed systems. For linear isotherm systems, simple algebraic equations are derived from the analysis to link product purity and recovery to zone lengths, bed movement velocity, flow rates, column capacity factors, and mass transfer coefficients (Ma and Wang, 1997). Once product purity and recovery are specified for a given system, the zone flow rates and bed movement velocity that provide the highest throughput and the lowest solvent consumption can be determined from the solutions. The study shows that in a given system, there is a tradeoff between product purity and throughput. Moreover, if bed volume and product purities are fixed, the longer the separation zone lengths, the higher the throughput. Dynamic simulations based on a detailed rate model that considers axial dispersion, film mass transfer, and intraparticle diffusion are developed and they are used to compare the column profiles and effluent histories of CMB and simulated moving bed (SMB). The comparison shows that the standing wave design equations derived for CMB systems are applicable to SMB systems with eight or more columns.

Based on these fundamental studies, Dr. Wang's group has proposed a systematic model-based design approach for SMB design (Wu et al. 1998). In this approach, isotherm and mass transfer parameters are first estimated from batch equilibrium tests, pulse tests, and frontal chromatography tests. These parameters are used in the standing wave analysis to generate zone flow rates and step time. Rate model simulation are then used to generate column profiles and effluent histories to make sure that product purities and yield are as expected from the standing wave analysis. A few pilot SMB experiments are carried out to obtain transient column profiles and effluent histories, which in turn are compared with the predictions from fate model simulations. This approach has been used successfully in designing SMB systems for sugar separations (Ma and Wang, 1997, Ma et al. 1998), amino acid separations (Wu, et al. 1997, Wu, et al. 1998), and pacitaxel purification (Wu, et al. 1999).

If isotherm and mass transfer parameters can be estimated accurately, the model-based design approach works well. However precise mass transfer parameters are difficult to obtain for some large scale SMB units. Dr. Wang's group has developed mass transfer design method for such cases (Xie, et al. 1999) In this method, effluent histories of SMB runs based on a design that does not consider mass transfer effects are obtained first. The breakthrough curves of the impurities indicate the propagation speeds of the impurity waves due to the mass transfer effects. Zone flow rates and switching time are modified according to the standing wave analysis to prevent the impurity concentration waves from reaching the product ports. Compared to the model-based

design, this method is simpler, requires little computation time and can be applied when mass transfer parameters are either unknown or inaccurate. Results from rate model simulations and pilot SMB experiments show that this method can improve product purity and can be implemented on line without restarting SMB runs. The results indicate a strong potential of this method for on-line control.

A well designed four-zone SMB can achieve a binary split of a mixture into a raffinate product and an extract product with high purity and high yield of both products. Separation of glucose from fructose is a well known example. Standing wave analysis can be used to show that a four-zone SMB can separate a three component mixture into two fractions. The highest affinity solute can be recovered as a pure extract product, while the two other solutes can be recovered together in the raffinate. A four-zone SMB can also recover the lowest affinity solute as a pure raffinate product and the two higher affinity solutes in the extract. However, the solute of intermediate affinity can not be recovered in pure form in a four-zone SMB using a continuous feeding and product withdrawal operation. Dr. Wang and her collaborators have shown recently that a nine-zone SMB which consists of two SMBs coupled in parallel (with the same step time) can achieve continuous separation of a three-component mixture of sulfuric acid, glucose, and acetic acid. All three components can be recovered with high purity (>98%) and high yield (>90%). The nine-zone SMB can also separate a four component mixture of sulfuric acid, glucose, xylose, and acetic acid, into three fractions if the two solutes of intermediate affinities (glucose and xylose) are recovered as one product. Experimental data using synthetic mixtures and biomass hydrolysate show that the standing wave analysis approach also works well for multicomponent separations. The column concentration profiles and product effluent histories are in close agreement with rate model simulations. This study shows that a combination of the standing wave analysis and rate model simulations significantly reduces the number of experiments needed in developing a robust nine-zone SMB with 19 design parameters (nine-zone lengths, nine-zone flow rates, and step time).

Publications

Wooley, R., Z. Ma, and N.-H.L. Wang, "A Nine-Zone Simulated Moving Bed for the Recovery of Glucose and Xylose from Biomass Hydrolyzate," *IEC Research, 37,* 3699-3709(1998).

Wu, D.J., Y. Xie, Z. Ma, and N.-H.L. Wang, "Design of SMB Chromatography for Amino Acid Separations," *I.E.C. Research, 37,* 4023-4035 (1998).

Ma, Z., T. Mallmann, B.D. Burris,and N.-H. L. Wang, "Standing Wave Design of Nonlinear SMB Systems for Fructose Purification," *AIChE J., 44,(12),* 2628-2646 (1998).

D.J. Wu, R. D. Whitley, Z. Ma, and N.-H. L. Wang, "Mass Transfer Effects in Dynamic Nonlinear SMB Systems," Proceedings of the 6th International symposium on Fundamentals of Adsorption, 461-466 (1998).

Jin, X., Z. Ma, J. Talbot, and N.-H.L. Wang, "A Model for the Adsorption Equilibria of Solutes with Multiple Adsorption Orientation," *Laugmuir, 15(9),* 3321-3333 (1999).

Wu, D.J., Z. Ma, and N.-H. L. Wang, "Optimization of Throughput and Desorbent Consumption in SMB Chromatography for Paclitaxol Purification," *J. of Chromatography, A, 855,* 71-89 (1999).

Hritzko, B.J., M.J. Ortis-Vega, and N.-H.L. Wang, "Adsorption of N-Phosphono methyliminodiacetic Acid, Iminodiacetic Acid, and Sodium Chloride on Poly-4-Vinylpyridine," *IEC Research*, in press.

Meeting Presentations

1998 AIChE Annual Meeting, Miami Beach, FL. Nov. 15-20. Symposium on Advances in Bioseparations: Adsorption and Chromatographic Separations, D.J. Wu (speaker), Z. Ma, and N.-H. L. Wang, "Design and Optimization of SMB Systems for Paclitaxel Purification."

1998 AIChE Annual Meeting, Miami Beach, FL., Nov. 15-20. Symposium on Adsorption and Other Processes for Dilute Solutions, B. Hritzko (speaker), Z. Ma, and N.-H. L. Wang, "A Carousel Process Based on Thermal Swing for the Separation of H- phosphonomethyl- iminodiacetic Acid and Sodium Chloride."

1998 Annual AIChE Meeting, Miami Beach, FL., Nov. 15-20. Poster Session: Fundamentals of Adsorption and Ion Exchange. B.Hritzko (presenter), Z. Ma, M. Ortiz-Vega, and N.-H. L. Wang, "Pore and Surface Diffusion Model of N-phosphonomethyliminodiacetic Acid and Iminodiacetic Acid on Poly (4-vinlypyridine)."

1998 Annual AIChE meeting, Miami Beach, Fl., Nov. 15-20. Poster Session: Recent advances in Application of Adsorption and Ion Exchange. K. Kauffman (presenter), Z. Ma, and N.-H. L. Wang. "Analysis, Dynamic Simulation and Animation of Simulated Moving Bed Chromatography for Large Scale Separation and Purification."

PREP 99, San Francisco, CA, May 6, 1999. R. Wooley (speaker), Z. Ma, and N.-H.L. Wang, "ine-Zone SMB for Ternary Fractionation."

Invited Lectures

"VERSE-Dynamic Simulations of Large-Scale Batch and Continuous Adsorption and Chromatography Processes," Westinghouse Savannah River Site, Aiken, NC, August 12, 1998.

"Fundamentals and Applications of Continous Chromatography for Biochemical Purification," Feb. 11, 1999, ADM, Decatur, IL 62521.

"Batch and Continuous Chromatography: Fundamentals and Applications," March 19, 1999, Merck, Rahway, NJ.

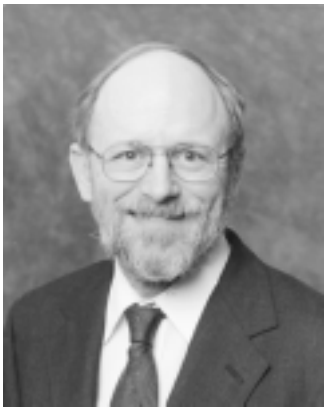
"An Overall Mass Transfer Design Method for SMB Chromatography for Amino Acids," PREP 99, San Francisco, CA. May 26, 1999.

"Simulated Moving Bed Chromatography: Fundamentals and Applications," Great Lakes Chinese American Chemical Society, Third Annual Conference, Arlington Heights, Il. August 28, 1999.

Phillip C. Wankat

1970

Clifiton L. Lovell Distinguished Professor of Chemical Engineering



Degrees

BS, Purdue University, 1966

PhD, Princeton University, 1970

MSEd, Purdue University, 1982

Interests

Adsorption and Chromatography

Distillation

Teaching Improvement

Awards and Major Appointments

Chair, Union Carbide Award Committee, ChE Division, ASEE, 1998-99

Inaugural Group, *Purdue University Book of Great Teachers*

Elected to Purdue Teaching Academy

Research Areas

New multicomponent gas adsorption cycles: New multicomponent gas separation methods which combine chromatographic operating methods with adsorbent regeneration cycles are being developed. These include elution chromatography cycles for dilute systems and displacement chromatography cycles for concentrated systems. Vacuum, pressure, steam and thermal swing regeneration methods are being explored. New methods for simulated moving beds (SMBs) are being developed.

Other research in progress: Methods to improve distillation and make it more energy efficient are being explored. Combined adsorption and reaction is being analyzed. Methods to increase the effectiveness and efficiency of teachers are under development.

Publications

Arumugam, B.K. and P.C. Wankat, "Pressure Transients in Gas Phase Adsorptive Reactors," *Adsorption, 4,* 345-354 (1998).

Arumugam, B.K., J.F. Banks and P.C. Wankat, "Pressure Effects in Adsorption Systems," *Adsorption,* (in press, 1999).

Arumugam, B.K. and P.C. Wankat, "Technical Note: Modified Operation of Isotachophoresis," *Separ. Sci. Technol., 33,* 1567-1570 (1998).

Wankat, P.C., "An Analysis of Articles in the Journal of Engineering Education", *J. Engr. Educ., 88,* 37-42 (1999).

Wankat, P.C., "Reflective Analysis of Student Learning in a Sophomore Engineering Course," *J. Engr. Educ. 88,* 195-203 (1999).

Wankat, P.C., and F. S. Oreovicz, "An Education Course for Engineering Graduate Students," Proceedings ASEE 1999 Annual Conference, PDF file 00161, (1999).

Wankat, P.C., "Effective, Efficient Teaching," Proceedings ASEE 1999 Annual Conference, PDF file 00167, (1999).

Wankat, P.C., "Educating Engineering Professors in Education," *J. Engr. Educ.* (in press)

Teaching Column Co-authored with F.S. Oreovicz in *ASEE PRISM:*

"What is Good Teaching?" September 1998, p. 16.
"Content Tyranny," October 1998, p. 15.
"Building Better Rapport," November 1998, p. 14.
"Some Assembly Required," December 1998, p. 14.
"Office Hours R_x," January 1999, p. 15.
"In Praise of Testing," February 1999, p. 18.
"Hit your Mark," March 1999, p. 18.
"Chart Your Course," April 1999, p. 18.

Editorial Boards

Separation and Purification Methods

Chemical Engineering Education, *Associate Editor*

Separation Science and Technology

Adsorption

Invited Lectures

"Teaching Efficiently and Well," Iowa State University, Ames, Iowa, February 11, 1999.

"Multicomponent Simulated Moving Beds," Advanced Separation Technology (AST), Lakeland, Florida, March 17, 1999.

"Multicomponent Simulated Moving Beds," Dow Chemical Company, Midland, Michigan, April 22, 1999.

Wankat, P.C., "Fame, Fortune or both: Life After Tenure," ASEE Annual Meeting, Charlotte, North Carolina, June 22, 1999. (Invited panelist)

Meeting Presentations

Gunaseelan, P. and P.C. Wankat, "Dynamic Sieve Tray Model for Pressure Transients During Start-Up of Absorbers," AIChE Annual Meeting, Miami Beach, Florida, November 19, 1998.

Wankat, P.C., "Syllabus and Course Goals," AIChE Annual Meeting, Miami Beach, Florida, November 17, 1998.

Wankat, P.C., "Effective, Efficient Teaching," AIChE Annual Meeting, Miami Beach, Florida, November 17, 1998.

Wankat, P.C. and F.S. Oreovicz, "An Education Course for Engineering Graduate Students," ASEE Annual Meeting, Charlotte, North Carolina, June 21, 1999.

Wankat, P.C., "Effective, Efficient Teaching," ASEE Annual Meeting, Charlotte, North Carolina, June 21, 1999.

Projects Funded

Award Amount	PI/Sponsor/Title	Project Period
$244,001.00	R.P. Andres National Science Foundation Electronically Linked Cluster Networks	08/97-07/00
$440,561.00	R.P. Andres R. Reifenberger National Science Foundation Cluster Based Probes for Nanostructure Analysis	08/95-06/99
$334,831.00	R.P. Andres Army Research Office Nanoelectronic Functional Devices: Architecture & Fabrication	09/96-02/00
$23,671.00	R.P. Andres Purdue Research Foundation Magnetic Thin Films	01/98-12/99
$251,000.00	O.A. Basaran NASA Forced Oscillations of Pendant and Sessile Drops	06/96-06/00
$783,033.00	O.A. Basaran DOE Fundamentals of Electric Field - Enhanced Multiphase Separations	08/96-07/00
$13,237.00	O.A. Basaran Purdue Research Foundation Drop Break-Up in Random Pressure Fields	05/99-04/00
$66,190.00	J.M. Caruthers MSU/ AFOSR Durability Characterization of High Temperature Polymer Matrix-Carbon Fiber Composites for Future Air Force Applications	03/98 - 11/99
$23,875.00	J.M. Caruthers Purdue Research Foundation Study of Viscoelastic Relaxation During Chemical Deg Radiation in Polymer Solids	01/98-03/00
$330,000.00	J.M. Caruthers Air Force Office of Scientific Research Solid State NMR Spectrometer for Studying Polyamide Matrix Resins	03/99-02/00
$59,703.00	J.M. Caruthers “Caterpillar, Inc.” Application of Artificial Intelligence Methods for the Formulation of Engineering Plastics and Rubbers	07/98-07/99
$82,502.00	J.M. Caruthers Air Force Office of Scientific Research Modeling and Lowering Residual Stresses in Bonded Composite Patch Repairs of Metallic Aircraft Structures	02/98-11/99

Award Amount	PI/Sponsor/Title	Project Period
$12,646.00	D.S. Corti Purdue Research Foundation Computer-Assisted Molecular Theories of Superheated Liquids	08/99-08/00
$90,000.00	W.N. Delgass Dupont Central Research & Development Research for Expanding the Horizons and Overall Understanding of Heterogeneous Catalysis	12/94-99/99
$12,005.00	W.N. Delgass Purdue Research Foundation Direct Vapor Phase Propylene Epoxidation over Gold Catalysis	1/99 - 12/99
$366,321.00	F.J. Doyle National Science Foundation An Integrated Approach to Environmentally Conscious Paper Mill Operations	10/97-10/00
$272,729.00	E.I. Franses National Science Foundation Adsorption and Surface Tension of Surfactant/Lipid/Protein Mixtures: Direct Probing of Surface Layers and Theoretical Modeling	03/97-03/00
$306,945.00	E.I. Franses Public Health Service Engineering Design of Novel Lung Surfactant Formulations	09/98-08/00
$20,000.00	J.A. Lauterbach American Chemical Society Non-Linear Phenomena During Heterogeneously Catalyzed Reactions Observed with Ellipsomicroscopy	09/97-09/99
$208,119.00	J.A. Lauterbach National Science Foundation Development of an Imaging FT-IR System for Combinatorial Sciences	09/98-09/00
$11,666.00	J.A. Lauterbach Purdue Research Foundation In Situ Microscopy of Dynamic Processes on Catalyst Surfaces	01/99-01/00
$141,310.00	J.A. Lauterbach National Science Foundation In Situ Microscopy and Spectroscopy of Dynamic Behavior	04/98-04/00
$48,000.00	J.H. Lee National Science Foundation Intelligent Model Based Control of Chemical Processes	08/98-02/00

Award Amount	PI/Sponsor/Title	Project Period
$69,243.00	J.H. Lee Auburn University / DOE "Energy Efficient Kraft Pulping for High Bleachable," Los Lignin Content Pulp	09 / 98-09 / 99
$50,000.00	J.H. Lee American Chemical Society Iterative and Adaptive Text Input Design for Multivariable System Identification	09 / 98-09 / 99
$13,237.00	J.H. Lee Purdue Research Foundation "An Integrated, Product-Quality Oriented Approach to " "Modellings, Estimations and Control of Batch" Processes	05 / 99-05 / 00
$24,530.00	J.F. Pekny National Science Foundation Foundations of Computer Aided Process Operations	8 / 99-8 / 00
$12,646.00	J.F. Pekny Purdue Research Foundation A Computationally Tractable Approach to Risk Based Supply Chain Management	08 / 99-08 / 00
$60,000.00	N.A. Peppas Showalter Trust Showalter Distinguished Professorship in Biomedical Engineering	11 / 93-06 / 00
$346,586.00	N.A. Peppas National Science Foundation IGERT: Training Program on Therapeutic and and Diagnostic Devices	08 / 99-08 / 01
$223,151.00	N.A. Peppas National Institute of Health PH Sensitive Complex Hydrogels for Protein Drug Release	07 / 99-6 / 00
$363,636.00	N.A. Peppas National Science Foundation Polymer / Mucin Adhesion for Targeted Therapy	09 / 97-08 / 00
$409,722.00	N.A. Peppas National Institute of Health Peg-promoted Mucoadhesive Drug Delivery Systems	08 / 97-08 / 00
$118,363.00	D. Ramkrishna University of Minnesota / NSF Cybernetic Modeling of Hybridoma Growth Under Glucose-Amino Acid Limitations	07 / 98-06 / 00

Award Amount	PI/Sponsor/Title	Project Period
$495,000.00	F.J. Doyle + 250,000 (in kind) “ J.F. Pekny G.V. Reklaitis V. Venkatasubramanian Computer Integrated Process Operations Center Individually Supported	05 / 96-99 / 99
$314,489.00	G.V. Reklaitis “Shell Companies Foundation, Inc.” Shell Oil Company Foundation Fellowship	09 / 85-12 / 99
$354,179.00	G.V. Reklaitis U.S. Department of Education Purdue Program for Graduate Assistance in Chemical Engineering Areas of National Need	08 / 98-08 / 00
$157,107.00	G.V. Reklaitis C.D. McAllister Endowment Goddard Fellowship	06 / 90-99 / 99
$48,600.00	G.V. Reklaitis National Consortium Graduate Minorities Engineering and Science National Consortium for Minorities Fellowship	07 / 98-07 / 99
$139,546.00	G.V. Reklaitis Advanced Process Combinatorics / ARO Use of Distributed Computing for the Application of Mathematical Programming to Batch Process Scheduling and Design	11 / 95-11 / 99
$60,551.00	G.V. Reklaitis USDA Developing Environmentally and Economically Sustainable Food Processing Systems	09 / 95-09 / 99
$213,600.00	E.M. Sevick-Muraca National Science Foundation National Young Investigator Biomedical Optical Imaging	09 / 94-03 / 00
$57,559.00	E.M. Sevick-Muraca Univ. of Vermont / NSF Recursive Bayesian Optical Tomography	09 / 98-09 / 00
$415,243.00	E.M. Sevick-Muraca Mallinckrodt Medical	08 / 94-01 / 00
$293,822.00	E.M. Sevick-Muraca National Science Foundation Characterization of Dense Particle Suspensions of Dense Particle Suspensions Using Frequency-Domain Photon Migration	05 / 99-05 / 02

Award Amount	PI/Sponsor/Title	Project Period
$355,872.00	E.M. Sevick-Muraca PHS-NIH National Cancer Institute Photon Migration Measurements for Tissue Diagnostics	07/95-07/00
$510,636.00	E.M. Sevick-Muraca Public Health Service-NIH Frequency-Domain Lifetime Spectroscopy: A Tissue Phantom Study	09/96-09/99
$145,335.00	E.M. Sevick-Muraca Army Research Office Fluorescence Lifetime Imaging for Breast Cancer Detection and Diagnostics	07/96-08/99
$93,563.00	J.L. Sinclair Univ. Of Arizona - DOE Optimization of Coal Particle Flow Patterns in Low Nox Burners	10/97-01/00
$10,000.00	J.L. Sinclair Sandia National Labs Investment of Kinetic Theory Modes of Turbulent Gas-Solid Flow	08/99-09/99
$12,005.00	J.L. Sinclair Purdue Research Foundation Detailed Non-Intrusive Flow Data in Dense-Phase Particle-Laden Systems	01/99-01/00
$23,807.00	V. Venkatasubramanian Purdue Research Foundation Automated Process Hazards Analysis of Batch Chemical Processing	09/97-03/00
$30,000.00	V. Venkatasubramanian “Honeywell, Inc.” Abnormal Situation Management	02/99-02/01
$195,351.00	V. Venkatasubramanian Lubrizol Corporation A Proposal to Develop a Neural Network-Genetic Algorithm Framework for Product Design and Formulation	12/95-12/99
$303,030.00	V. Venkatasubramanian National Science Foundation Process Systems Tools for the Development and Management of Environmentally and Economically Conscious Manufacturing	09/95-09/99
$39,536.00	N.-H.L. Wang Westinghouse Savannah River/DOE WSRC Ion Exchange Data Review	08/98-09/99

Award Amount	PI/Sponsor/Title	Project Period
$162,436.00	N.-H.L. Wang Abbott Laboratories "Model-based Design, Optimization, and Scale-up of" Simulated Moving Bed Chromatography for Antibiotics Recovery and Purification	08/97-08/00
$126,833.00	N.-H.L. Wang GIST-Brocades Applications & Modifications of Verse for Process "Design, Optimization and Scale up."	05/98-05/00
$24,970.00	N.-H.L. Wang Purdue Research Foundation Thermal Fractionation in Continuous Chromatography	05/98-05/00
$55,623.00	N.-H.L. Wang Dow Chemical Company Feasibility Studies of a Novel Continuous Adsorption Technology for Separating Organic Acids from a Dow Waste Stream	12/98-12/99
$98,120.00	N.-H.L. Wang Lilly and Company Feasibility Studies of SMB Size Exclusion Chromatography for Insulin Purification	05/99-05/00
$55,556.00	P.C. Wankat National Science Foundation New Regeneration Methods for Adsorption	09/97-09/99
$55,556.00	P.C. Wankat National Science Foundation New Regeneration Methods for Adsorption	09/97-09/99
$24,767.00	P.C. Wankat Purdue Research Foundation Latent Heat Regeneration of Adsorbers	03/98-03/00
$211,952.00	P.C. Wankat National Science Foundation Multicomponent SMB/Chromatographic Separations	07/99-07/02

Thesis Projects

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Buss, Michael Richard *Andres*	Characterization of Fragile Nanostructures Using Scanning Force Microscopy	PhD August 7, 1998
*Gerogianni, Dimitra *Pekny & Reklaitis*	Incorporating Risk Analysis in the Solution of Process Management Problems: Knapsack Substructures	MS August 7, 1998
Ortiz-Vega, Melvin *Wang*	Thermal Swing Adsorption for the Separation of Two Amino Acids	MS August 7, 1998
*Pryor, Seqwana Nichole Thomas *Delgass*	Structural Characteristics and Catalytic Activity of Promoted Raney Nickel Catalysts for Selective Hydrogenation of Butyronitrile	PhD August 7, 1998
*Wen, Xinyun Franses	Tension and Solution Behavior of Aqueous Soap and Gemini Cationic Surfactants	MS August 7, 1998
*Bonilla, Griselda Lauterbach	A Time-Resolved FTIR Study of the Dynamics of CO Oxidation Over a Silica Supported Pt Catalyst	MS December 19, 1998
*Green, Karen Elizabeth Lauterbach	The Adsorption and Photopolymerization of Methyl Methacrylate and Acrylic Acid on Pt(110) Using Time-Resolved FT-IRAS and Temperature-Programmed Desorption	MS December 19, 1998

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Honkomp, Steven Joseph *Pekny/Reklaitis*	Solving Mathematical Programming Planning Models Subject to Stochastic Task Success	PhD December 19, 1998
Kauffman, Kenneth James *Wang*	Analysis of Simulated Moving Bed Size Exclusion Chromatography	MS December 19, 1998
Kayihan, Arkan *Doyle*	Local Nonlinear Control of a Process Actuator	MS December 19, 1998
*Podual, Kairali *Doyle/Peppas*	Glucose-Sensitive Cationic Hydrogels for Insulin Release	PhD December 19, 1998
Stavens, Kevin Bruce *Andres*	Distributed Arc Cluster Source for Production Capture of Refractory Metal and Bimetallic Clusters	MS December 19, 1998
Foss, Aaron Cooper *Peppas*	Controlled Release of 5-Fluourouracil from Hydrogels.	MS May 8, 1999
*Hassan, Christie Marie Dorski *Peppas*	Structure and Morphology of Poly(vinyl alcohol) Gels Prepared by Freezing and Thawing Processes	PhD May 8, 1999
Notz, Patrick K. *Basaran*	Dynamics of Drop Formation in an Electric Field	MS May 8, 1999
Samikoglu, Omer *Pekny & Reklaitis*	Evolutionary Programming Based Analysis of theCritical Parameters of Combinatorial Optimization Problems.	MS May 8, 1999

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Sundaram, Ananthapadmanaban *Venkatasubramanian*	Design of Engineering Materials Using Hybrid Neural-Networks and Evolutionary Algorithms	PhD May 8, 1999
*Torres-Lugo, Madeline *Peppas*	Novel pH-Sensitive Hydrogel for the Oral Delivery of Salmon Calcitonin	MS May 8, 1999
*Vedam, Hiranmayee Venkatasubramanian	Op-Aide: An Intelligent Operator Decision Support System for Diagnosis and Assessment of Abnormal Situations in Process Plants	PhD May 8, 1999
Wu, Dingjun *Wang*	Design of Simulated Moving Bed Chromatographic Processes for Biochemical Purification	PhD May 8, 1999

Course Offerings and Seminars 1998-1999

Course Offering - Fall 1998

Class	Course Title	Instructor	Enrollment
200	Chem. Engr. Seminar	Squires	130
201,301,401	Co-op Seminar	Squires	93
205	Chem. Engr. Calculations	Sinclair	118
211	Intro. to Chem. Engr Thermo.	Lauterbach	51
303	Chem. Engr. Honor Seminar	Pekny	9
306	Design of Staged Separation	Wang	124
348	Chem. Reaction Engineering	Andres	34
377	Momentum Transfer	Basaran	108
378	Heat and Mass Transfer	Kessler	34
400	Professional Guidance	Squires	117
434	Chem. Engr. Laboratory I	Muench, Eckert, Houze	108
456	Process Dyanmics & Control	Pekny	119
461	Biomedical Engineering	Hannemann	30
496	Chem. Engr. Honors Lab	Delgass, Muench	5
540	Transport Phenomena	Greenkorn	12
557	Intelligent Systems	Vankatasubramanian	14
558	Rate Control Separ. Proc.	Wankat	21
597A	Risk Mgmt. Proc. Develop.	Blau, Pekny	20
597T	Biochemical Engineering	Tsao	69
610	Advanced Chem. Engr. Thermo	Peppas	19
620	Transport Phenomena I	Sevick-Muraca	25
630	Applied Math. for Chem. Engr.	Caruthers	25
633	Prob. Method in Chemical Engr	Ramkrishna	10
666	Methods of Catalysis	Delgass	16
668	Colloid Interfacial Ph.	Franses	10
690	Chemical Engr. Seminar	Relkaitis	88
697A	Polymer Science and Engr.	Caruthers, Peppas	12

Special Projects:

411	Chem. Engr. Science. Research Projects	23

Course Offering - Spring 1999

Class	Course Title	Instructor	Enrollment
201,301	Co-op Seminar	Squires	51
205	Chem. Engr. Calculations	Kessler	49
211	Intro. to Chem. Engr Thermo.	Franses	100
300	Chem. Engr. Seminar	Squires	112
320	Statistical Modeling & Qual. Enhan.	Blau	148
348	Chem. Reaction Engineering	Peppas	79
377	Momentum Transfer	Greenkorn	41
378	Heat and Mass Transfer	Houze	86
430	Principles of Molecular Engr.	Andres	127
435	Chem. Engr. Laboratory I	Muench, Eckert, Wang	118
442	Chemistry and Engr. of High Poly.	Caruthers	58
450	Design and Anal. of Proc. Systems	Reklaitis, Tsao, Venkatasubramanian	126
597C	Polymer Science Engr. Lab	Caruthers	10
597M	Adv. Chem E. Measmnt Lab	Lauterbach	13
597S	Particulate Systems	Sinclair	25
611	Advanced Topics Che Thermodynamics	Corti	3
621	Transport Phenomena II	Basaran	23
656	Advanced Process Control	Lee	7
660	Chem. React Engr.	Ramkrishna	23
690	Chem. Engr. Seminar	Reklaitis	84
697E	Biomedical Optical Engineering	Sevick-Muraca	6

Special Projects:

411	Chem. Engr. Science Research Project	31
412	Chem. Engr. Design Research Project	3
499	Research in Chemical Engineering II	7

Speaker	Title	Date
Professor Michael Loewenberg Chemical Engineering Department Yale University New Haven, CT 06520-2159	Drop Breakup in Viscous Flows	September 10, 1998
Professor Fernando J. Muzzio Chemical & Biochemical Engineering Department Rutgers University Piscataway, NJ 08855-0909	A Fundamental Approach to Mixing and Segregation of Granular Materials	September 17, 1998
Professor Diane Hildebrandt Chemical Engineering Department University of the Witwatersrand Johannesburg, South Africa	The Attainable Region Approach to Optimisation	September 24, 1998
Professor Juergen Kueppers Experimentalphysik III Universitaet Bayreuth and Max-Planck-Institut fuer Plasmaphysik, Garching, Germany	Atom-adsorbate Reactions: Eley-Rideal and Hot-atom Processes	October 22, 1998
Dr. Jon Siddal Research Leader Corporate Research Catalysis Lab 1776 Building Midland, MI 48674	Industrial Polymer Process Development	November 5, 1998
Prof. Douglas M. Ruthven Chemical Engineering Department University of Maine Orono, ME 04469-5737	Diffusion in Zeolites	December 3, 1998
Dr. Robert Burchfield R&D Director Lilly Corporate Center Eli Lilly & Company Indianapolis, IN	To be announced	December 10, 1998

Spring 1999

Speaker	Title	Date
Professor Rena Bizios Department of Biomedical Engineering Rensselaer Polytechnic Institute Troy, NY 12180	Frontiers in Cellular/Tissue Engineering	January 19, 1999
Professor John Y. Walz Chemical Engineering Department Yale University New Haven, CT 06520-2159	Control of Colloidal Stability Using Nonadsorbing Polyelectrolytes	January 28, 1999
Professor Michael J. Miksis Engineering Sciences & Applied Math 2145 Sheridan Road Northwestern University Evanston, IL 60208	Dynamics of a Drop on a Thin Liquid Film	February 11, 1999
Professor Kristi S. Anseth Chemical Engineering Department University of Colorado Boulder, CO 80309-0424	Novel Orthopaedic Biomaterials Based on Crosslinkable Polyanhydrides	February 18, 1999
Professor L.S. Fan Chemical Engineering Department Ohio State University Columbus, OH 43210-1180	Particle and Bubble Dynamics in Gas-Liquid-Solid Fluidization	February 25, 1999
Professor E. Daniel Blankschtein Chemical Engineering Department Massachusetts Institute of Technology Cambridge, MA 02139-4307	Predicting Surfactant Solution Behavior from Molecular Structure	March 25, 1999
Professor Joe Qin Department of Chemical Engineering University of Texas, Austin Austin, TX 78712-1062	Between Open-Loop and Closed-Loop Control: Multivariate Process Monitoring	April 1, 1999
Mr. Mark Cassells Global Technology Leader Ag Chemicals Process Research & Operations Dow Chemical Co. 1710 Building Midland, MI 48640	To be Announced	April 8, 1999

Speaker	Title	Date
Professor George Stephanopoulos Department of Chemical Engineering Massachusetts Institute of Technology Cambridge, MA 02139	To be Announced Kelly Lecture	April 22-23, 1999
Professor Kyu-Yong Choi Chemical Engineering Department University of Maryland College Park, MD 20742-211	On the Modeling and Control of Industrial Polymerization Reactors	April 29, 1999