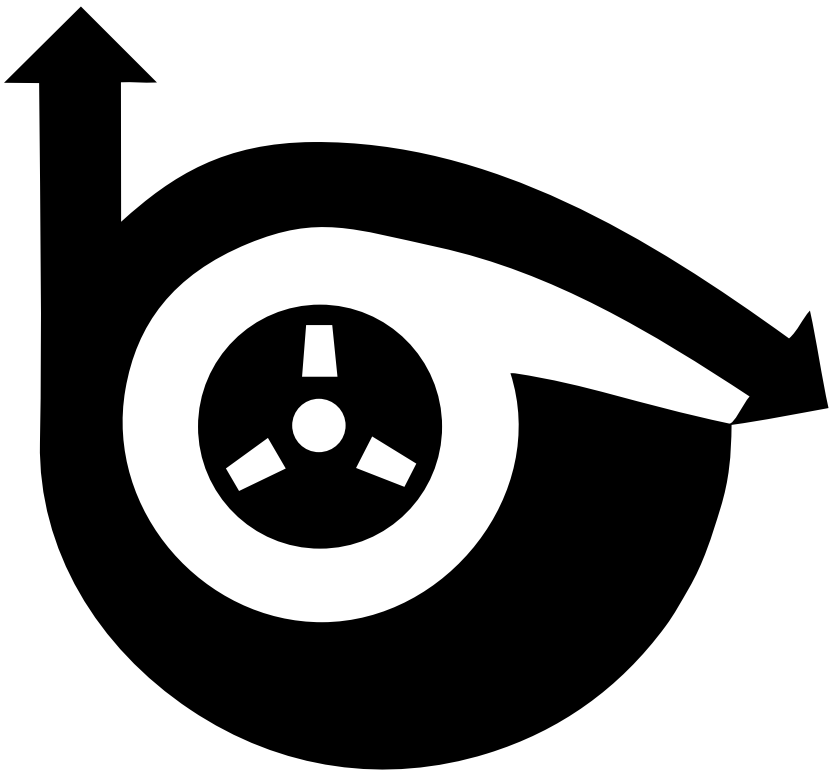
The School of Chemical Engineering

Annual Report

July 1, 1994 - June 30, 1995



Purdue University

West Lafayette, Indiana

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Frank Oreovicz, editor; Carolyn Blue, compiler
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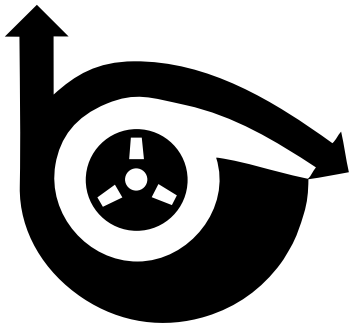


1994-1995

Academic Year Highlights

The School of Chemical Engineering

Faculty Affairs

Faculty Appointments

In August, 1994, Dr. Eva Sevick-Muraca joined the School as Assistant Professor, after three years teaching experience on the faculty at Vanderbilt University. Dr. Sevick's research expertise lies in theories and measurements of light propagation through condensed heterogeneous matter with applications in biomedical engineering and process on-line monitoring applications. She is a 1993 NSF Young Investigator and this year was selected to be the Purdue Engineering nominee for the Presidential Faculty Fellow competition. Shortly before the close of this academic year, it was announced that Professor Sevick-Muraca was the recipient of a National Institutes of Health Research Career Development Award, a very prestigious five year award with funding beginning in July, 1995.

During this year, the School attracted to our faculty Dr. Osman Basaran, who was group leader and senior development staff member in the Chemical Technology Division of Oak Ridge National Laboratory. Dr. Basaran joined our faculty in July, 1995. His expertise lies in fluid mechanics and transport phenomena with emphasis on multiphase flow systems involving bubbles, drops, jets, atomization, and coating phenomena. He is both highly accomplished in mathematical modeling of such phenomena and in experimentation. Prior to his ORNL appointment he served as Senior Research Engineer with Air Products & Chemicals. His BS ChE is from MIT (1978) and PhD is from the University of Minnesota (1984). He joined the faculty as full professor without tenure.

Additional faculty appointments this year included the advancement of Professor Robert Greenkorn to Slayter Distinguished Professor of Engineering, and Professors Takoudis and Venkatasubramanian to the rank of full professor. Professor John Wiest left the faculty to take a position at the University of Alabama. Professor Alden Emery concluded his fifth year under the early partial retirement program of the University and retired in May, 1995 after 41 years on the faculty.

Professional Recognition

Faculty recognitions achieved this year included Professor Nicholas Peppas receiving AICHE outstanding paper and session awards for his contributions to the AICHE annual meeting. He also was awarded the 1995 APV Medal for his contributions to pharmaceuticals research at the 7th International Conference on Pharmaceutical Technology held in Budapest May 9-11, 1995. Professor Robert Squires received the Catalyst Award for outstanding teaching of the Chemical Manufacturers Association and the 1995 ASEE Chester F. Carlson Award for dis-

tinguished accomplishments of an educational nature on the basis of his pioneering educational simulated industrial experiment modules. Professor Frank Doyle was 1995 winner of both the Shreve Outstanding Teaching Award of the School and the A. A. Potter Award for Excellence in Teaching. He was also selected as the Engineering nominee for the 1995 Packard Fellowship. Professor D. Ramkrishna served as Melchior Visiting Professor at the University of Notre Dame in Fall, 1994, and as a visiting professor at the Jawaharlal Nehru Centre for Advanced Scientific Research in India in Summer 1994. He also was named UDCT Diamond, a distinguished alumnus award of the University of Bombay. Professor Reklaitis was elected Fellow of AIChE.

Several of the faculty accepted new editorial board appointments in the past year. Emeritus Professor Lyle Albright was named to the Board of *Polymer News.* Professor Peppas was appointed to the editorial board of *Tissue Engineering*, while continuing as editor of Biomaterials and serving as editorial board member for eight other journals. Professor Sevick-Muraca was named to the Editorial Advisory Committee of the Biomedical Optics Journal of the Optical Society of America.

Professional Activities

During 1994, two books which Professor Peppas co-edited appeared in press: *Biomaterials for Drug and Cell Delivery* and *Superabsorbent Polymers: Science and Technology*. In addition, two others are undergoing publication: *Biopolymers II* (Advances in Polymer Science) and *Polymer/Inorganic Interfaces* (MRS). Professors Greenkorn and Kessler submitted for press their revised and updated textbook, *Basics of Momentum, Heat, and Mass Transfer.*

The expertise of the faculty continues to be recognized through appointments to various professional committees, panels, and boards. Professor Jim Caruthers was appointed to the Standing Committee on Program and Technical Review of the U.S. Army Chemical and Biological Defense Command, National Research Council. Professor Elias Franses was named to the External Advisory Committee of the NSF EPSCOR Center of the University of Kentucky in the Research cluster on Biofunctional Membranes. Professor Reklaitis was elected to the Governing Board of the Council for Chemical Research. Professor Sevick-Muraca was appointed to the Biotechnology Resource Advisory Committee of the Beckman Laser Institute and Medical Clinic in Irvine, California.

Professor Delgass was named to the Executive Committee of the Organizing Committee for the 11th International Congress on Catalysis, to be held in 1996 and to the Technical Program Committee for the 15th North American Meeting of the Catalysis Society, 1997. Professor Lackritz was appointed to the International Advisory Committee for the joint American Chemical Society/Optical Society of America Symposium on Thin Films for Photonic Applications. She will serve as Program chair for the 1995 Portland meeting and as Symposium Organizer for the 1998 Orlando meeting. Professor Doyle was chosen to serve on the Technical Program Committee for the Fifth Chemical Process Control Conference, January, 1996, a specialist conference which is held once every five years. Professor Pekny was elected chair of Area 10c: Computers in Operations and Information Processing of the National Programming Committee of AICHE and was named co-chair

of the 3rd International Symposium of Foundations of Computer Aided Process Operations. This week-long specialists conference, which is also held once every five years, is planned for July, 1998. Professor Venkatasubramanian served as co-chair of the International Conference on Intelligent Systems in Process Engineering, held in July, 1995, and was member of the International Advisory Board for the 9th International Conference on Artificial Intelligence Applications in Engineering, held in Toulouse, France.

Collectively, the faculty served as organizers, chairs, or members of advisory committees for over thirty conferences and symposia. For instance, Emeritus Professor Albright was chair of the symposium, "Nitration" held at the ACS , Anaheim Meeting in April. Professor Doyle chaired sessions on process control at both the AIChE Annual Meeting in San Francisco and at the ACC meeting in Seattle. Professor Lackritz chaired a session on electrically and optically active polymers at the American Physical Society Meeting while Professor Peppas served as chair of a session on biomedical polymers in Japan. Professor Sevick-Muraca was chair of the session on lasers in medicine and science at the Conference of Lasers and Electro-Optics of the Optical Society of America. The faculty of the School again chaired a total of ten sessions at the November, 1994 AIChE Annual Meeting.

Our faculty is widely recognized for its technical expertise as evident from the 80 invited lectures and seminars which they gave at conferences and academic as well as industrial sites in all parts of the world. Professor Andres presented a lecture at the DOE Workshop on Research Needs Assessment for Future Use of Nanofabricated Materials. Professor Caruthers was plenary lecturer at the ACS 17th Biennial Polymer Symposium, while Professor Doyle served as panelist at the Neural Information Processing Systems Workshop in Vail, Colorado. Professor Franses was invited lecturer at the International Workshop *Bubble and Drop 1995* held in Italy. Professor Ramkrishna lectured at the Engineering Foundation Conference: Biochemical Engineering IX in Davos, Switzerland while Professor Reklaitis participated in the invited Memorial Session to David Rippin which took place at the ESCAPE 5 Meeting in Slovenia. Professor Sevick-Muraca was plenary lecturer at the Eastern Analytical Conference in New York; Professor Venkatasubramanian gave the keynote lecture at the 2nd IFAC International Conference on AI/KBS in Process Control held in Lund, Sweden, and Professor Wang lectured at the 13th International Symposium on Preparative Chromatography. Professor Wankat presented a live NTU lecture which was broadcast via satellite to over 75 sites across the country.

Staff Affairs

In January of this year, Dr. Wayne Muench joined the School of Chemical Engineering as director of instructional laboratories. Dr. Muench, who earned a PhD from Purdue in Organic Chemistry (1973), has over 20 years of industrial R&D experience with Dow Chemical and Great Lakes Chemical, including management of significant bench and pilot scale product and process development projects. This experience, coupled with his expertise in R&D safety programs, will serve him well in strengthening and revitalizing the laboratory component of our instructional program.

At the close of this year, Mrs. Katie Eckman, who has served the School for many years, most recently as Undergraduate Program Administrator, entered the early partial retirement program offered by the University. Under this program, she will assume half-time duties for a period of up to 5 years. Over the many years in which the undergraduate office has been in her charge, she has devoted herself totally to the needs of our undergraduate students. Her caring, energetic efforts have been highly appreciated by the students and have been recognized by a number of university-wide awards. Ms. Lisa (Burge) Bunch (BS ChE '87), who worked for Eli Lilly for six years as a staff engineer as well as the Department of Freshman Engineering, has been chosen as Mrs. Eckman's successor. In the Spring of this year, the School also had to seek a replacement for the CHME building deputy, Mr. Jerry Haugen. After a search of some three months, a successor was found in Mr. Jeff Valley. During the interim period of some three months, Mr. Richard Lowe, our Electronics Technician served as acting building deputy in an exemplary fashion.

Graduate Education and Research

Research Productivity

The research productivity of the faculty and research staff remained at high levels during the past year as measured by funding, proposal activity, publications, and conference presentations. Total research expenditures, including funds from federal, industrial, and unrestricted sources was at the level of $4.33 million, exceeding the $4.01 million level of 93-94 and $3.6 million levels of 1992-93. The 8% increase is notable given the tight federal and private research environment. These totals exclude general fund expenditures as well as the separately budgeted activities of the Laboratory for Renewable Resources Engineering. This level of research expenditures was sustained by significant proposal writing efforts: 63 new proposals were submitted and 39 awards obtained, compared to 55 and 51 in the previous year. Total new awards totaled $2.7 million plus an additional $0.3 million in minor accounts. New award totals declined from the level of $3.63 million of the previous year, in large measure due to delays in award processing by two federal sponsors which will shift these awards into the next academic year. Unrestricted grants, gift funds, and gifts in kind declined somewhat to a total of $1.27 million from the previous year level of $1.36 million.

The tangible results of the intense research effort of the faculty and research staff included nearly 230 refereed papers in various stages of the publication process as well as an additional 40 submitted and under review. These totals compare well with 220 and 50 reported in 1993-94. The faculty and their research groups contributed 110 conference paper presentations during this year, nearly equaling the level of 120 attained in the previous year. When combined with the 80 invited lectures, this level of activity translates to an average of over nine lectures and conference presentations per active research faculty member. Given the record high enrollments which the School has sustained over the past year with the attendant high demands of teaching and student mentoring, the level of research and professional activity is indeed very high.

Graduate Program

Fall 1994 graduate enrollments declined modestly by design from 136 in the previous year to 128, reflecting in part the reduction in Department of Education GAANN fellowships. In 1994-95, the School graduated 21 PhD and 20 MS students, compared to 20 and 16 in the previous year. Of the 20 MS degree recipients, 13 are continuing for the PhD. These graduation rates are likely to sustain our position among the top four US chemical engineering programs in annual PhD awards. In Fall 1995, we expect to admit 24 new graduate students, including three minority and seven international students. This compares with the class of 25 which entered the program in Fall 1994 and included seven minority and eight international students. The employment prospects for graduate degree candidates has improved somewhat from last year. Nonetheless, at the time of the awarding of their degrees, two MS and three PhD awardees were still seeking employment. In all cases these were international students.

The Graduate Student Organization of the School conducted the third annual Chemical Engineering Graduate Research Symposium on August 18, 1994. The program featured formal presentations by 22 students in two parallel sessions as well as a poster session in which the work of more junior research students was exhibited. Sixteen CPI companies were represented and these representatives served as the jury for the selection of the best presentations. The Fourth Symposium is scheduled for August 17, 1995 and is expected to involve representatives from 14 companies.

Instruction

Awards

The high quality of the instructional program of the School is the result of the combined efforts of the faculty, the graduate teaching assistants and the support staff. The fine contributions of the teaching assistants were recognized through the 1995 Purdue University Magoon Awards which Rob Crane and Steve Honkomp received. Chris Brazel was selected by the seniors for the Award for Teaching Excellence in the Undergraduate Laboratory.

The 1995 student awards voted by the faculty were announced at the annual Razz Banquet. The Junior awards went to Jennifer Harting, who won the Stephen Craig Award, and Melissa Laucks, the George T. Tsao Award. Among the seniors, Michele Bland won the Omega Chi Epsilon Award; Jeffrey Lander the Lottes Award, while the American Institute of Chemists Award was given to Nicole Lark. The AIChE Outstanding Senior Award was presented to Lisa Ingamells. The annual Senior Design Project Award, given to the student team which produces the best design for a longer term case study executed in the senior process design course, was shared by the design group of Michele Bland, Edward Crane, and Dennis Willig. The second place team consisted of Jennifer Cook, James Wagler, and Kerri Wilkinson.

Enrollment Trends

In Fall 1994 the School reached its historical peak in fall undergraduate enrollments with 676 students. This occurred despite the imposition of a 2.9/4.0 grade point based cap on transfers of students who had completed the Freshman Engineering program. Even under the cap, the ChE sophomore class numbered 182 students. This year the School also experienced its largest ever graduating class, totaling 185

students over the August, December, and May graduations. This should sustain our position as the number one ChE program in number of BS graduates. With the continued application of the cap, we expect the total enrollments to decline to 610 in Fall, 1995. This number would remain about 100 students above our target enrollments for a faculty of 24, four of whom have significant administrative responsibilities outside of the School. Under present circumstances, it proved necessary to again offer a section of the senior laboratory course in the summer session in order to avoid having to schedule Saturday or evening laboratory sessions during the Fall semester.

The employment prospects for the 1995 class improved somewhat from the low state which had been reached in the previous year. At the time of the May graduation, 42% of BS graduates did not have firm job or graduate school commitments. This is an improvement over the 46% recorded in the previous year. Nonetheless the average starting salary did increase by 2.3%. The May graduating class consisted of 43% women; 34% of the graduates had completed the cooperative education program. Only 16% of the coops had no firm commitments upon graduation.

Honors and Undergraduate Research Programs

The faculty's efforts to provide our undergraduate students with research and extended duration independent research project experience continue to grow. In the 1994-95 academic year 34 seniors completed the Honors BS program, compared to 28 in the previous year. The Honors program involves a more challenging senior laboratory course, a one year bachelor's thesis research project, and several selected elective courses. The faculty were again successful in obtaining renewal of two NSF Research Experience for Undergraduates grants. One these, under the direction of Professors Franses and Wiest, provided support for ten students, while the second, led by Professor Takoudis, provided support for ten students and involved collaboration with faculty from Materials and Electrical Engineering. Furthermore, about 80 juniors and seniors took advantage of independent projects courses with the faculty over the past year. These projects involve undergraduates working with graduate students and faculty on specific research projects and thus facilitate one-to-one student-faculty contact. Of course, this commitment of faculty time comes in addition to normal teaching and mentoring duties and thus reflects the strong dedication which the faculty have to educating undergraduates.

Facilities Development

The major facilities renovation project which took place during this year was the remodeling of 2,600 square feet of laboratory space intended for two instructional laboratories - the Dow Advanced Instrumentation Lab and the Polymer Science and Engineering Laboratory - and two laboratories associated with Professor Peppas' research group. This remodeling project was funded with $337,000 obtained under an NSF Facilities Renovation Grant and equal matching funds committed by the University. This project was completed in early June, 1995. The Instrumentation and Polymers laboratory courses which employ these laboratories will be offered in the next academic year.

A second remodeling project involved the preparation of a laboratory for Professor Sevick-Muraca. This project was completed in September, 1994 under funding provided by the Dow Chemical Company.

Industrial & Alumni Relations

The School's New Directions Program continues to be quite active. With the addition of NALCO to the membership, the total of New Directions partner companies stands at 20. The Industrial Advisory Council to New Directions met in annual meeting on September 9-10, 1994 to review the status of the School's academic programs in preparation for the 1995 ABET accreditation visit. Two of the new initiatives for the 1994-95 academic year were the development of a plan for the renovation and re-equipment of the Undergraduate Laboratory which was to be undertaken by the Facilities Committee and the development of a plan for improving recruitment and retention of minority students, graduate and undergraduate, which was to be undertaken by the newly formed Diversity Committee. These activities are currently in progress. Two members were elected to the Executive Committee of the New Directions Program. These are Mike Ramage, recently promoted to President of Mobil Technology Corporation, and Bill Smith, Executive Director, Engineering and Manufacturing, Eli Lilly. The Executive committee met March 15 and again on June 21 to review the School's progress in meeting the objectives of its current five year plan. The next meeting of the Industrial Advisory Council was held on September 22-23, 1995.

Alumni Awards

In Spring 1995, two candidates from among the alumni of the School were awarded Distinguished Engineering Alumnus Awards during the annual DEA program which took place Gala Weekend. These awardees were Dr. Che-I Kao, Chief Scientist and Research Fellow, of the Dow Chemical Company (MS '66 and PhD '68), and Robert Postlethwait, President Central Nervous System Business Unit, Eli Lilly and Company (BS '70).

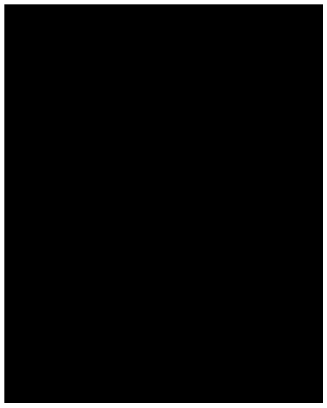
Three alumni were selected to receive 1995 Outstanding Chemical Engineer Awards: Dr. William Eykamp, President of Abcor, Inc. (ret.) (BS '58); Dr. Craig McLaughlin, President of Texaco Development Corporation, (BS '68, MS '70, PhD '72); and William Smith III, Executive Director, Engineering and Manufacturing services, Eli Lilly and Company (BS '69). These awards are presented during the course of individual visits to the campus which include seminars which the recipients give to our students and staff. The School is very proud to number among its alumni individuals of such distinguished accomplishment.

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

Mechanism and kinetics of isobutane alkylation

Coke formation during pyrolysis

Gasification and liquefaction of coal

Publications

Albright, L.F., "Comments on Alkylation of Isobutane with Ethylene: A Thermodynamic Study," *Ind. Eng. Chem. Research, 33*, 3274-3276 (1994).

Albright, L.F., "Nitration," *Kirk-Othmer Encyclopedia of Chemical Technology*, Vol. 17, 1995.

Albright, L.F. and Lang, E.G., "Regeneration of Used Sulfuric Acid," *McKetta Encyclopedia of Chemical Processing and Design*," Vol. 52, 1995.

Editorial Board

Encyclopedia of Chemical Processing and Design (1976-present).

Polymer News (1995).

Invited Lectures

Six local chapters of American Institute of Chemical Engineers.

Chaired Conferences/ Symposia

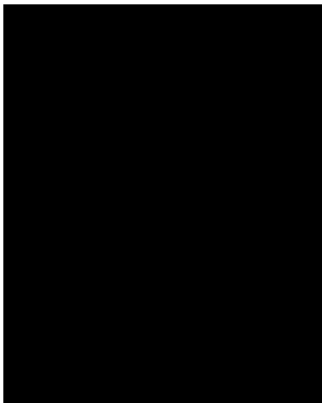
Chairman of Symposium, "Nitration," American Chemical Society, Anaheim, CA, April 2-5, 1995.

** 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
Optoelectronics
Catalysis

Research Areas

Electronic Conduction in Molecular Nanostructures: The development of sophisticated techniques for semiconductor film growth has made it possible to fabricate layered semiconductor films with layer thicknesses as small as 2 nm. These quantum well structures have been the focus of intense research activity during the last decade and many useful applications have emerged. It has long been recognized that a whole new generation of devices might become feasible if material could be patterned laterally with a precision comparable to that afforded in the vertical direction by film growth techniques. It seems clear, however, that such nanometer-sized structures will have to be fabricated out of metals rather than semiconductors since a semiconductor particle with dimensions of ~ 1 - 10 nm has hardly any carriers. Unfortunately, the granularity of metal films makes it difficult to "chisel out" useful structures with nanometer dimensions. We are pursuing a complementary approach to this problem at Purdue in collaboration with a multidisciplinary group from Physics, Chemistry, and Electrical Engineering. We propose to fabricate nanostructure films by interconnecting preformed metal clusters, that have uniform diameters in the 1 - 10 nm size range, by means of conductive polymers. A coupled nanostructure device can then be made by patterning such films supported on an insulating substrate.

Synthesis of Ultrafine Particles and Measurement of Particle-Particle and Particle-Substrate Interactions: Ultrafine particles or clusters having diameters in the nanometer size range have unique size-dependent electronic and physical properties. Polycrystalline solids produced by consolidating nanoscale powders also exhibit unique properties such as greater hardness, higher yield strength, and improved processing characteristics over coarse grain materials. While a scientific understanding of the reasons for the novel properties of small clusters and cluster-assembled materials is gradually being

achieved, several critical engineering issues remain largely unaddressed. Two of the most important of these issues are the focus of our research: (1) techniques for synthesizing nanometer particles at high production rates and low cost and (2) measurement of particle-particle and particle-substrate interactions for nanoscale particles. We have developed a series of aerosol techniques for cluster synthesis that show promise for economical, large-scale, cluster production. We are also measuring the forces exerted by nanoscale clusters by means of an atomic force microscope (AFM) and are attempting to develop a comprehensive picture of the important issues governing particle interaction and adhesion in the nanometer size range.

Fabrication of Novel Nanostructured Solid Materials and Films: Two critical parameters that characterize small clusters are their size and their chemical composition. Self-assembly of the particles in the gas phase provides a means of partially controlling both of these parameters. As cluster size becomes larger than a few atoms, however, the number of possible isomeric configurations a cluster may assume grows exponentially and the atomic configuration or structure of the cluster becomes important. Furthermore, while techniques exist which enable the synthesis of novel metal, semiconductor and insulator clusters and their physical characterization with unprecedented precision, much in the way of process technology must still be developed. It is one thing to identify a cluster with desirable physical or chemical properties in a cluster-beam experiment, but quite another to devise a practical process by which this unique ultrafine particle can be used to construct a film or solid material.

We have discovered that metal clusters can be thermally annealed as free particles in the gas phase to assume a minimum energy structure and that the annealed clusters can be captured in an organic solvent to form stable colloidal suspensions. The key to the latter process is use of a surfactant species, which forms a self-assembled monolayer around the clusters and prevents them from coagulating. These surfactant coated clusters can then be assembled into ordered solid materials and films. Several novel catalytic and optoelectronic materials have been synthesized in this way.

Publications

Purcell, S.T. Vu Thien Binh, N. Garcia, M.E. Lin, R.P. Andres, and R. Reifenberger, "Field Emission from Narrow Bands above the Fermi Level of Nanometer Scale Objects, *Phys. Rev. B, 49,* 17259 (1994).

Chao, L.C. and R.P. Andres, "Synthesis of a Supported Metal Catalyst Using Nanometer-Size Clusters," *J. Colloid Interface Sci., 165,* 290 (1994).

Lin, Shihcher T. and R.P. Andres, "Adhesion of Nanoscale Metal Clusters to Semiconductor Surfaces: A Scanning Tunneling Microscopy Examination," *Mat. Res. Soc. Symp. Proc., 317,* 149 (1994).

Bielefeld, J. D. and R.P. Andres, "The Microstructure and Electrical Resistivity of Cluster-Based Thin Films," *Mat. Res. Soc. Symp. Proc., 317,* 155 (1994).

Patil, A.N., R.P. Andres and N. Otsuka, "Synthesis and Minimum Energy Structure of Novel Metal/Silica Clusters," *J. Phys. Chem., 98,* 9247 (1994).

Paithankar, D.Y., J. Talbot, and R.P. Andres, "Molecular Dynamics Simulation of the Elastic Deformation of Nanometer Diameter Metal Clusters," *Mat. Res. Soc. Symp. Proc.*, 332, 99 (1994).

Patil, A.N., N. Otsuka, and R.P. Andres, "Synthesis and Characterization of Structured Metal/Silica Clusters," *Mat. Res. Soc. Symp. Proc.*, 332, 195 (1994).

Mahoney, W., D.M. Schaefer, A.N. Patil, R.P. Andres, and R. Reifenberger, "Substrate Induced Deformation of Nanometer-Size Gold Clusters Studied by Non-Contact AFM and TEM," *Surf. Sci.*, 316, 383 (1994).

Invited Lectures

Oxide Encapsulated Metal Clusters as Novel Oxidation Catalysts," DOE Workshop on Research Needs Assessment for Future Use of Nanofabricated Materials in Energy Applications, M.I.T., December, 1994.

Meeting Presentations

"A Comparison of the Growth Process and Electrical Properties of Neutral-Cluster-Based and Thermally-Evaporated Thin Metal Films," AIChE 1994 Annual Meeting, San Francisco, CA, November, 1994.

"The Synthesis of Nanometer-Sized Metal Clusters and Metal Cluster-Assembled Quantum Dot Arrays," AIChE 1994 Annual Meeting, San Francisco, CA, November, 1994.

"The Formation of Nanoscale Clusters by Gas Phase Aggregation of Metal Atoms Using Arc Evaporation," AIChE 1994 Annual Meeting, San Francisco, CA, November, 1994.

"Encapsulated Silver Clusters as Oxidation Catalysts," Fall 1994 MRS Meeting, Boston, MA, November, 1994.

"A Comparison of the Physical Properties of Cluster-Based and Vacuum-Evaporated Thin Metal Films," Fall 1994 MRS Meeting, Boston, MA, November, 1994.

"Probing the Nucleation of a Thin Film on an Atomically Flat Substrate," Fall 1994 MRS Meeting, Boston, MA, November, 1994.

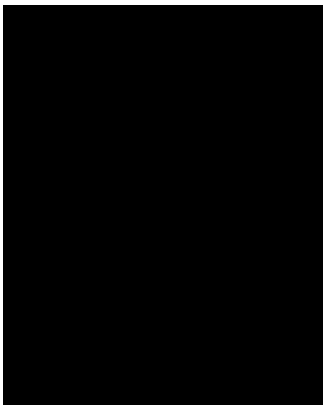
"Aerosol Synthesis of Nanoscale Clusters Using Atomspheric Arc Evaporation," Fall 1994 MRS Meeting, Boston, MA, November, 1994.

"Encapsulated Silver Clusters on Oxidation Catalysts," ACS Meeting, Anaheim, CA, April, 1995.

James M. Caruthers

1977

Professor



Degrees

SB (Chem), Massachusetts Institute of Technology, 1975

SM, Massachusetts Institute of Technology, 1975

PhD, Massachusetts Institute of Technology, 1977

Interests

Viscoelasticity of solids

Polymer rheology

Structure-property relationships in polymers

Composites

Awards and Major Appointments

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

Research Areas

A more complete understanding of the engineering properties of amorphous polymers in the glass transition region is a research area that we have been addressing over the last several years. Polymers are usually processed in the fluid state, solidified by being cooled through the glass transition region, and then used in the solid state. The flow prior to solidification and the details of the solidification process can substantially alter the engineering properties in the solid; thus, an understanding of the mechanical behavior for complex thermal and deformation histories in the glass transition region is of considerable importance. We have recently measured the creep response to large applied loads (i.e. like those used in molding and forming operations) in the glass transition region. The data indicate that large loads can substantially accelerate the rate of viscoelastic relaxation, and the rate of relaxation decreases upon removal of the load. These data provide the first definitive experimental evidence that stress influences the rate of viscoelastic relaxation as well as affects the nonlinear stress strain relationship. Also the linear and nonlinear viscoelastic behavior is being measured while the load and temperature are both being changed. These are the first definitive nonisothermal experiments, and they indicate that the traditional method of calculating the nonisothermal response as a series of isothermal responses can be significantly different from the experimentally measured nonisothermal viscoelastic behavior. This understanding of the nonisothermal, nonlinear viscoelastic behavior has important implications for the manufacture of polymeric components, since all polymer processing operations are

nonisothermal. Using the Rational Thermodyanmics framework, the group has developed a nonlinear constitutive equation incorporating a deformation dependent material time to describe the nonlinear and nonisothermal experiments described above as well as (i) specific volume relaxation in the glass transition region, (ii) yield in tension and compression, and (iii) the effect of temperature and deformation rate on the linear and nonlinear mechanical behavior.

A second major research area is the investigation of the fundamental molecular motions that are responsible for density, thermal, and mechanical relaxation at the glass transition. Series of poly(phenylenes), poly(carbonates), and poly(sulfones) with systematic changes in the chemical structure have been synthesized along with the monomeric and dimeric analogues. The mechanical relaxation near T_g is being studied dilatometrically for these materials, and the thermal relaxation near T_g is being studied by differential scanning calorimetry. The molecular motions that give rise to the observed volume and heat capacity relaxation are being studied via ^{13}C and ^{2}H solid state NMR; specifically, we are probing how changes in chemical structure effect a variety of rotational motions along the mainchain backbone. In conjunction with Prof. Wiest, we are also using molecular dynamics methods to calculate the molecular motions for glass forming polymers with simple chemical structures. These theoretical predictions about the types of motion will be compared to those measured experimentally with the solid state NMR.

The third research is the development of methods for the prediction of a variety of engineering properties of polymers from chemical structure. These activities include implementation of the more traditional group contribution methods, application of modern equation-of-states for polymer solids and solutions, and development of neural networks for prediction of polymer properties. Along with Profs. Chao and Venkatsubramanian we are working with the AIChE Design Institute for Physical Properties Research (DIPPR) to develop and verify the best methods for predicting the transport properties of polymer solids and solutions required in numerous design calculations. Recent results have shown that the application of (i) modern equation-of-states for polymers and (ii) the pattern recognition capabilities of neural network can effect an order-of-magnitude improvement in the prediction of selected z properties of engineering polymers. The development of improved predictive methods for the properties of polymers and polymer solutions can have significant implications in the design of polymer manufacturing processes.

Publications

Venkatasubramanian, V., K. Chan and J.M. Caruthers, "Computer-Aided Molecular Design Using Genetic Algorithms," *Computers in Chemical Engineering*, 18, 833 (1994).

Kim, D.J., J.M. Caruthers, N.A. Peppas, and E. VonMeerwall, "Self- and Mutual-Diffusion Coefficients in the Dodecane/Polystyrene System," *Journal of Applied Polymer Science*, 51, 661 (1994).

Sy-Siong-Kiao, R., K.C. Chao, and J.M. Caruthers, "Polymer Chain-of-Rotators Equation of State," *Proceedings International Symposium on Thermodynamics in Chemical Engineering and Industry*, Beijing, China, (1994).

Venkatsubramanian, V., K. Chan, and J.M. Caruthers, "Genetic Algorithmic Approach for Computer-Aided Molecular Design," *ACS Symposium Series, No. 589*, 396 (1995).

Ramakrishnan, R., J.F. Pekny, and J.M. Caruthers, "A Combinatorial Algorithm for Effective Generation of Long Maximally Compact Lattice Chains," *J. Chemical Physics* (in press).

Sy-Siong-Kiao, R., J.M. Caruthers, and K.C. Chao, "Polymer Chain-of-Rotators Equation of State,"*Industrial Engineering Chemistry Research* (in press).

Novenario, C.R., J.M. Caruthers, and K.C. Chao, "A Mixing Rule to Incorporate Solution Model into Equation of State," *Industrial & Engineering Chemistry (*in press).

Invited Lectures

"Application of Chemistry Fundamentals for Manufacturing and Lifetime Performance of Engineering Polymers," ACS 17th Biennial Polymer Syposium, Polymers in Critical Technologies, American Chemical Society, San Juan, Puerto Rico, November, 1994.

"Application of Artificial Intelligence Methods for the Design of Polymer Systems," Lubrizol Corporation, Cleveland, OH, June, 1995.

"Models for the Prediction of VLE Behavior and Other Thermophysical Properties for Engineering Materials," Department of Mechanical Engineering, Purdue University, West Lafayette, IN, June, 1995.

"Application of Artificial Intelligence Methods for the Design of Polymer Systems," Lord Corporation, Cary, NC, June, 1995.

"A Nonlinear Time-Dependent Constitutive Equation for Engineering Polymers," NSF Institute for Materials and Mechanics, Workshop on Constitutive Behavior in Engineering Plastics, La Jolla, CA, June, 1995.

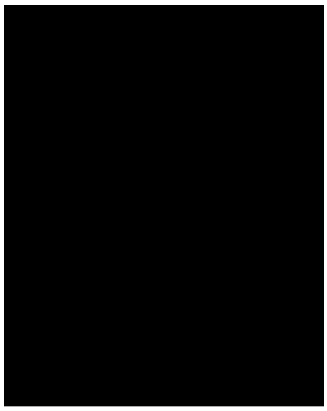
Meeting Presentations

"Nonlinear Viscoelastic Relaxation in the Glass Transition Region," ASME Summer National Meeting, Los Angles, CA, June, 1995.

Kwang-Chu Chao

1968

Harry Creighton Peffer Professor Emeritus of Chemical Engineering



Degrees

BS, National Chekiang University, 1948

MS, University of Wisconsin, 1952

PhD, University of Wisconsin, 1956

Interests

Thermodynamics

Statistical Mechanics

Fluid Phase Equilibria

Research Areas

Thermodynamic properties of polymer melts and solutions: An equation of state has been developed by focusing on the oscillatory motion of the segments of a polymer molecule. The Polymer Chain-of-Rotators equation has been found to give an account to generally within 0.1% of the specific volume of polymers for which extensive data are available over a substantial temperature range at pressures to several hundred MPa. Correlations are developed for the three equation parameters with the structural elements of the repeating segment of the polymer molecule so that estimates can be made of the thermodynamic properties of a polymer from its chemical structure. The equation of state is applied to the description of phase equilibrium of mixtures of polymers.

Molecular Simulation of Fluid Phase Equilibria: The objective of the research is to develop methods for the molecular simulation of fluid phase equilibrium based on molecular structure and intermolecular forces. A new method of molecular simulation of free energy has been developed for calculation with the canonical ensemble and the isothermal isobaric ensemble. A new method for the direct simulation of vapor-liquid equilibrium using the semi-grand ensemble, is investigated.

Publications

Peng, Chun-Lan and Kwang-Chu Chao, "Vapor-Liquid Equilibrium in Binary Mixtures of n-Heptane + Ethyl ter-Butyl Ether," *Am. Inst. Chem. Eng.*, New York, NY, DIPPR Data Series No. 2, pp. 18-22 (1994).

Peng, Chun-Lan and Kwang-Chu Chao, "Vapor-Liquid Equilibrium in Binary Mixtures of Ethyl Ter-butyl Ether + Ethanol and Butyraldehyde + n-Propanol," *Am. Inst. Chem. Eng*, New York, NY, DIPPR Data Series No. 2, pp. 23-27 (1994).

Chen, Ai-Qi, George J. Urbanus, and Kwang-Chu Chao, "A New Vapor-Liquid Equilibrium Cell and VLE Data for Mixtures of 1-Propanol and p-Xylene," *Fluid Phase Equilibria, 94,* 281-288 (1994).

Sysiogkiao, R., J.M. Caruthers, and K.C. Chao, "Polymer Chain-of-Rotators Equation of State," *Ind. Eng. Chem. Res*. (submitted).

Jin, Zhangli, Robert A. Greenkorn, and Kwang-Chu Chao, "Correlation of Vapor-Liquid Equilibrium Ratio of Hydrogen," *AIChE Journal, 41,* 1602-1604 (1995).

Watson, B.S., R.A. Greenkorn, and K.C. Chao, "Meta Stable and Unstable Fluid States by Molecular Simulation and Simulated States for Lennard-Jones Fluid, Ethane, n-Butane, and Water," *AIChE Journal* (submitted).

Novenario, C., J.M. Caruthers, and K.C. Chao, "A Mixing Rule to Incorporate Solution Model into Equation of State," *Ind. Eng. Chem. Res.*, (accepted).

Bereolos, Peter, Julian Talbot, and Kwang-Chu Chao, "Simulation of Free Energy without Particle Insertion in the NPT Ensemble," *Molecular Physics* (submitted).

Bereolos, Peter, Kwang-Chu Chao, and Julian Talbot, "Molecular Simulation of Fluid Phase Equilibria of Mixtures," *AIChE Journal* (submitted).

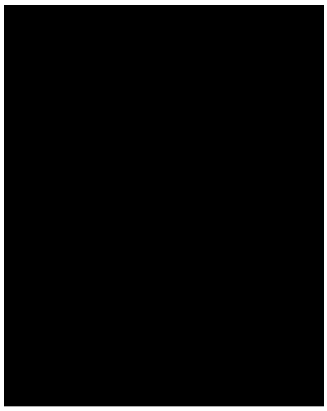
Meeting Presentations

"A Mixing Rule to Incorporate Solution Model into Equation of State," Am. Chem. Soc. Meeting, Anaheim, CA, April 5, 1995.

W. Nicholas Delgass

1974

Professor



Degrees

B.S.E., Chemical Engineering, University of Michigan, 1964

B.S.E., Mathematics, University of Michigan, 1964

M.S., Stanford University, 1966

Ph.D., Stanford University, 1969

Interests

Heterogeneous catalysis

Selective hydrogenation over Raney nickel

Partial oxidation - epoxybutene

Nitric oxide reactions

Solid acid catalysts

NMR, XPS, FTIR

Research Areas

Effects of metal particle size on Ethylene and Butadiene Epoxidation over Silver: Silver is unique among the elements in its ability to catalyze the reaction of oxygen with ethylene to form ethylene oxide rather than the thermodynamically preferred product, CO_2. It has also been shown recently to catalyze oxidation of butadiene to 3,4 epoxy 1-butene. The objective of Will Walters' work is to examine the effect of particle size and cesium chloride promotion on the catalytic behavior of Ag in these epoxidation reactions. Our particular interest is to use the transient response to an isotopic switch of $^{18}O_2$ for $^{16}O_2$ during steady state reaction to probe the nature of the kinetically significant oxygen species. The approach has been developed on unsupported Ag catalysts, where it shows the presence of a subsurface oxygen pool and, in some cases, the need to include a surface carbonate pool as well as an active surface oxygen pool in a model to describe the measured, time-dependent concentrations and yield the individual rate constants. Preliminary data suggest that the subsurface oxygen pool in the supported silver is substantially larger than that of macroscopic crystalline silver. Current work includes using ^{133}Cs NMR as a tool for following cesium promotion.

NMR of Sugars in Zeolites: This collaborative effort with Professors Tsao and Grutzner (Chemistry) brings together elements of biotechnology, catalysis, and NMR. Enzymatic conversion of cellulosic material to ethanol can provide a path for production of fuels from renewable resources, but this family of multistep processes has a number of bottlenecks. Hydrolysis of cellobiose to glucose is glucose inhibited,

for example, and xylose cannot be directly fermented to ethanol. Since hydrolysis of sugar polymers and isomerization of sugars are known to occur in strongly acidic solutions, this group is exploring the role that solid acid catalysts might play in cellulose conversion. Recent work uses ^{1}H and ^{13}C NMR to confirm the entry and reaction of glucose and xylose in zeolites.

^{13}C NMR studies have shown that glucose populates rigid bound, hopping, and mobile states in Y zeolite, depending on the degree of filling of the cavities. In the smaller channels of ZSM-5, glucose dehydrates to anhydroglucose. Current work by Jia Lee shows that ZSM-5 converts 2,3 butane diol to methyl ethyl ketone at temperatures below 200∞C and to substituted aromatics at higher temperatures. These studies are part of an ongoing effort to develop solid acid catalysts for environmentally sound production of chemicals, fuels and fuel additives.

VO-Zeolites as Catalysts for the Selective Catalytic Reduction of NO: Vanadium catalysts used commercially for removal of NO from stack gas have the remarkable property that they produce N_2 from NO and NH_3 even in the presence of oxygen. Using materials prepared in Professor Bein's laboratory in Chemistry, Bob Adams is investigating effects of vanadium oxide structure on this catalytic activity by isolating vanadium oxo species with fixed nuclearity in the supercages of the zeolite. Characterization of the materials by ^{51}V MAS NMR and diffuse reflectance spectroscopy shows that tetrahedral, octahedral, and/or square pyramidal coordination of V are all possible within the supercage and that the structures are stable up to 350°C at vanadium loadings up to 4 per cage and adsorb NH_3 strongly. The catalytic activity per vanadium does not diminish at the lowest vanadium loading, suggesting that sites containing only one vanadium atom are active in the zeolite matrix.

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, Tom Manz and Seqwana Thomas are studying the effects of alloy preparation and surface composition on the selective hydrogenation of butyronitrile to butylamine. Reactions in solution at atmospheric pressure and in neat butyronitrile at high pressure will test effects of alloy composition, annealing, leaching and post-activation promotion on selectivity to butyl- versus dibutylamine. We collaborate with Professors Trumble and Gaskell in Materials Engineering on the production of the alloys and control of the grain size and phase distribution. X-Ray photoelectron spectroscopy provides the surface composition information.

Publications

Tolia, A.A., R.J. Smiley, W.N. Delgass, C.G. Takoudis, and M.J. Weaver. "Surface Oxidation of Rhodium at Ambient Pressures as Probed by Surface-Enhanced Raman and X-Ray Photoelectron Spectroscopies." *J. Catal., 150,* 56-70 (1994).

Smiley, R.J. and W.N. Delgass, "XPS and SEM Characterization of PAN-based Carbon Fibers Treated in Oxygen and Nitric Oxide Plasmas." *Mat. Res. Soc. Symp., 318*, 361-366 (1994).

Eshelman, L.M. and W.N. Delgass, "Acetonitrile Synthesis over Potassium-Promoted, Supported Iron Catalyists," *Catalysis Today, 21,* 229-242 (1994).

Smiley, R.J. and W.N. Delgass, "Angle resolved X-Ray Photoelectron Spectroscopy Characterization of Plasma-Treated Pan-Based Carbon Fibers," *Surf. and Interface Anal.* (submitted).

Wen, J.Q., J.B. Grutzner and W.N. Delgass, "The structure, Dynamics and Acid Catalyzed Isomerization of Sugars on HY Zeolite Cavities — A Solid State ^{13}C and ^{2}H NMR Study," *J. Am. Chem. Soc.* (submitted).

Editor

Journal of Catalysis.

Invited Lectures

"Reaction and Mobility of Sugars in Zeolites," Catalysis Club of Chicago, Evanston, IL, December 5, 1994.

Chaired Conferences/ Symposia

Organizing and Executive Committee, 11th International Congress on Catalysis, Baltimore, MD, June, 1996.

Technical Program Committee, 15th North American Meeting of the Catalysis Society, Chicago, IL, May, 1997.

Meeting Presentations

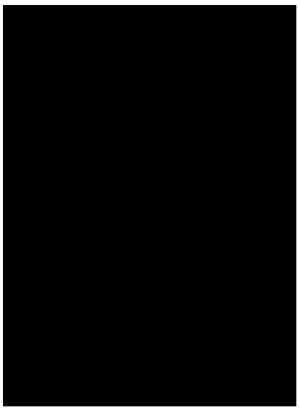
"Entry and Reaction of Sugars in Zeolites," AIChE National Meeting, San Francisco, CA, November 15, 1994.

"Methyl Ethyl Ketone and Substituted Benzenes from 2,3 Butanediol over Zeolite Catalysts," 14th North American Meeting of the Catalysis Society, Snowbird, UT, June 13, 1995.

Francis J. Doyle, III

1992

Assistant Professor



Degrees

B.S.E., Princeton University, 1985

G.P.G.S., Cambridge University, 1986

Ph.D., California Institute of Technology, 1991

Interests

Nonlinear Process Control

Biological Control Systems

Awards and Major Appointments

National Science Foundation National Young Investigator Award (1992).

R. N. Shreve Prize, Chemical Engineering Teaching Award (1994-95).

A.A. Potter Award, Engineering Teaching Award (1994-95).

Research Areas

Nonlinear Process Modeling and Control: Our work in this area covers 4 key issues: (i) identification of nonlinear process models, (ii) design of nonlinear model predictive controllers, (iii) low order nonlinear model construction, and (iv) analysis of control -relevant process nonlinearity. In the identification area, we have developed practical algorithms for parameter estimation of the coefficients in a Volterra series and related model structures. Application studies include biological reflexes and complex industrial polymerization reactors. These models are employed in model-based control schemes (MPC), where it has been found that they yield substantially improved performance over linear MPC. The control structure can be decomposed into linear and nonlinear contributions, suggesting an "operator-friendly" implementation scheme. On the model reduction theme, we have developed simple wave propagation models of distributed parameter systems for use in nonlinear model-based control schemes. Present studies have focused on the application of this approach to a complex distillation column, in which we employ input-output linearization for controller synthesis and an extended Kalman filter for parameter updating. The strength of this approach is the fact that the low order model consists entirely of physically meaningful states and parameters. The final project area, control-relevant nonlinearity analysis, has involved the construction of computational tools which indicate the degree to which a given process requires nonlinear compensation. The tool will find application in process design and in control structure determination, where "control-relevant" properties, as opposed to "open-loop" properties are critical.

Biosystems Analysis and Control: In this project, we have focused on biological representations of neurons for use in process modeling. In particular, we have returned to Hodgkin-Huxley type neuron models and are using nonlinear model reduction to synthesize meaningful building blocks. The end goal is to derive networks which use such neurons in a parsimonious fashion to model dynamic processes. This is in direct contrast to current approaches to neural network modeling which employ static computational elements, and attempt to capture dynamics through times series approaches which require a large number of parameters and record keeping of past input values. Initial efforts have focused on neuron types found in a particular biological regulatory system (blood pressure control) in an attempt to extract meaningful qualitative trends from the ionic channel dynamics. These analysis will serve a two-fold purpose: i) provide new tools for process technology, and ii) elucidate the control mechanisms in biological systems. These project is one part of a larger research program which seeks to develop an in depth understanding of a biological control system and its ramifications for engineering control principles. A second theme in this area is the modeling and analysis of controlled drug delivery devices from the perspective of advanced model-based control design. The key element in this approach is a detailed, physiologically accurate, model of the glucose-insulin system. An objective of this work is the formulation of a naturalistic objective function for the control system (cf. engineering metrics such as ISE). We are also working on the development of novel drug delivery devices—intelligent hydrogels. From a control perspective, these devices can approximate the dynamic behavior necessary to achieve the targeted delivery of insulin.

Publications

Henson, M.A., B.A. Ogunnaike, J.S. Schwaber, and F.J. Doyle III, "The Baroreceptor Reflex: A Biological Control System with Applications in Chemical Process Control," *Ind. & Eng. Chem. Res.*, 33, 2453-2466, (1994).

Doyle, F.J. III, H.M. Budman, and M. Morari, "Theoretical and Practical Aspects of Nonlinear Packed Bed Reactor Control," *Ind. & Eng. Chem. Res.*, (submitted) 1994.

Kwatra, H., R.D. Braatz, F.J. Doyle III, J.S. Schwaber, "Parameter Error Space for Hodgkin-Huxley Models Using A Nelder Mead Algorithm," *Biol. Cybernetics.* (submitted) 1994.

Aoyama, A., F.J. Doyle III, V. Venkatasubramanian, "Control-Affine Neural Network Approach for Nonlinear Non-minimum Phase Process Control," *J. Process Control* (submitted) 1994.

Doyle, F.J. III, T.A. Ogunnaike, and R.K. Pearson, "Nonlinear Model-Based Control Using Second Order Volterra Models," *Automatica*, 31, 697-714 (1995).

Doyle, F.J. III, F. Allgöwer, and M. Morari, "On Nonlinear Systems with Poorly Behaved Zero Dynamics," *IEEE Trans. Aut. Control* (in press) 1995.

Doyle, F.J. III, J. Hobgood, "A Practical Approach to Approximate Input-Output Linearization," *J. Process Control* (in press) 1995.

Bassett, M.H., P. Dave, F.J. Doyle III, G.K. Kedva, J.F. Pekny, G.V. Reklaitis, S. Subrahmanyam, D.L. Miller, M.G. Zentner, Perspectives on Model Based Integration of Process Operation," *Comp. Chem. Eng.* (in press) 1995.

Aoyama, A., F.J. Doyle III, V. Venkatasubramanian, "Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control," *J. Process Control* (in press) 1995.

Aoyama, A., F.J. Doyle III, V. Venkatasubramanian, "Adaptive Fuzzy Neural Network Approach for Nonlinear Process Control," *Eng. Appls. of AI* (submitted) 1995.

Pearson, R.K., T.A. Ogunnaike, and F.J. Doyle III, "Structurally Constrained Second-Order Volterra Models," *IEEE Trans. Accoustics and Signal Processing* (submitted) 1995.

Invited Lectures

"Reverse-Engineering Biological Control Systems for Applications in Process Operations," Arizona State University, Tempe, AZ, October, 1994.

"Novel Control Techniques from Biological Inspiration," panelist at Neural Information Processing Systems (NIPS) Workshop, Vail, CO, December, 1994.

"A Biologically Motivated Dynamic Nonlinear Scheduling Algorithm for Control," GM Research Center, Warren, MI, March, 1995.

"Opportunities for Process Control through Neuromimetics: the Reverse Engineering of Biological Reflexes," University of Michigan, Ann Arbor, MI, March, 1995.

Chaired Conferences/ Symposia

Session Chairman "Advances in Process Control," AIChE Annual Meeting, San Francisco, CA, November, 1994.

Session Organizer & Chairman "Modeling and Control in Biomedical Systems," American Control Conference, Seattle, WA, June, 1995.

Meeting Presentations

"A Model Reduction Scheme for a Pulp Digester," presented at AIChE Annual Meeting, San Francisco, CA, 1994.

"Approximate Linearized Control for a Fluidized Bed Reactor," presented AIChE Annual Meeting, San Francisco, CA, 1994.

"A Biologically Motivated Scheme for Nonlinear Process Modeling," presented at AIChE Annual Meeting, San Francisco, CA, 1994.

"Control-Relevant Identification for Volterra Model Predictive Control," presented at AIChE Annual Meeting, San Francisco, CA, 1994.

"A Control-Relevant Metric for Process Nonlinearity," Proc. American Control Conference, Seattle, WA, June, 1995.

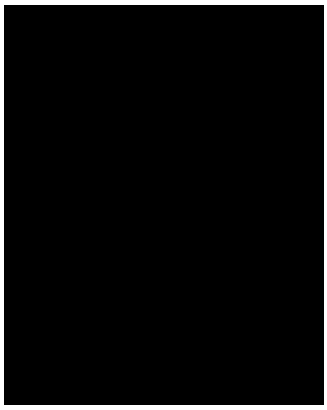
"Low-order Modeling for Nonlinear Process Control," Proc. American Control Conference, Seattle, WA, June, 1995.

"Control & Modeling of Drug Delivery Devices for the Treatment of Diabetes," Proc. American Control Conference, Seattle, WA, June, 1995.

Roger E. Eckert

1964

Professor and Director of the Undergraduate Program



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, statistical 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.

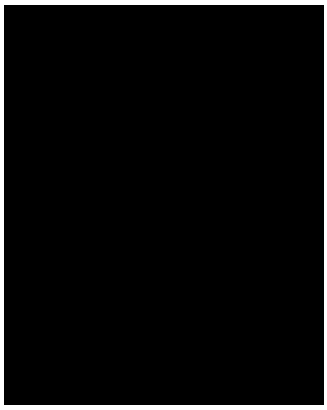
Polymer Flow Properties at High Shear Rates: Flow properties of viscoelastic polymers are being measured in novel and standard equipment with the ultimate objective of predicting those properties from chemical and physical structure. Emphasis is on the use of continuous flow devices with channels approximating 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.

Elias I. Franses

1979

Professor



Degrees

DEng. National Technical University, Athens, 1974

PhD, University of Minnesota, 1979

Interests

Adsorption equilibria and dynamics of surfactants and proteins at interfaces

Engineering design of lung surfactant formulations

Transport and ion exchange in thin organic films

Infrared spectroscopy and ellipsometry of monolayers and thin films

Awards and Major/ Appointments

Outstanding Paper Presentation Award, 85th.

American Oil Chemists Society Annual Meeting, Atlanta, Georgia, May (1994).

Editor, Colloids and Surfaces: A. Physicochemical and Engineering Aspects.

Canvassing Committee for the ACS Award in Colloid and Surface Chemistry, American Chemical Society (1993-1996).

External Advisory Committee, NSF-EPSCOR, University of Kentucky, October (1994), Research Cluster on Biofunctional Membranes.

Research Areas

Dynamic Adsorption of Surfactants and Proteins at Air/Water Interfaces. This phenomenon affects foam stability and foam-based separations of dilute solutions, coating flows, and the ability of lung surfactants to stabilize the alveoli during breathing. The lack of proper quantity or quality of lung surfactants is the cause of the respiratory distress syndrome of premature infants and adults suffering from major pulmonary diseases. In the past three years, we have made major advances concerning the physicochemical basis of the low surface tensions of aqueous lung surfactants. We have established the thermodynamic and mass transfer requirements for effective lung surfactants using a combination of experiment and theory. We are now working toward a better understanding of the colloidal requirements, i.e., the roles of surfactant particles structure, size, and morphology, and also of the molecular requirements of effective molecules. We are studying a variety of soluble surfactants, insoluble surfactants and lipids, and proteins using (i) a pulsating bubble surfactometer, (ii) two Langmuir balances and Langmuir-Blodgett apparatus; and (iii) a variety of other tension-measuring devices. We have built a oscillating jet instrument

for measuring dynamic surface tensions at milliseconds time scale, and are building an interferometer for probing of dynamic concentration profiles in interfacial mass transfer, and a radiotracer detector for probing adsorption at air/water interfaces. The research will focus on interfacial interactions of molecules of different sizes, for which we are developing novel comprehensive mathematical models for adsorption equilibria and dynamics.

Composition and Orientation of LB Film: We have developed the first detailed model of ion adsorption on Langmuir monolayers of fatty acids. The model has been tested with data of ionic compositions of transferred Langmuir-Blodgett (LB) films. The films have been analyzed with the use of detailed FTIR spectroscopy. In addition, new theory and methodology have been developed for determining orientation of molecular groups and chains by polarized FTIR-ATR (attenuated total reflection) spectroscopy. The method of LB deposition followed by FTIR has also been used to obtain composition and density information of mixed monolayers of lung surfactants for the preceding project. Finally, the structure of certain important polymer films, PMMA (polymethyl-methacrylate) and PHMA-AS (polyhexylmethacrylate-azobenzene sulfone) has been studied by detailed FTIR spectroscopy. The LB processing method has been compared with the more traditional spin-coating method. Such films are used for microelectronic or nonlinear device applications. These studies are continuing with the use of spectroellipsometry for more detailed characterization of thickness, structure, refractive index, and anisotropy.

Transport and Ion Exchange in Thin Organic Films. We have studied water transport in ultrathin films of cadmium stearate, PMMA, and PHMA-AS, and related it to the film microstructure. Detailed data and modeling revealed multidimensional transport through defects and through hard-to-permeate regions. Ion exchange dynamics was transport-limited. Data were obtained with in-situ infrared spectroscopy, with which the film structure was also monitored along with the transported species. The results have important implications for the barrier or membrane properties of ultrathin films and for the potential uses of LB films as ion sensors or ion-exchange materials. Current studies aim at understanding the roles of different ions and permeants, and in controlling the transport properties via improved processing methodology.

Publications

Sutandar, P., Ahn, D.J., and Franses, E.I., "FTIR ATR Analysis for Microstructure and Water Uptake in Poly(methylmethacrylate) Spin Cast and Langmuir-Blodgett Thin Films," *Macromolecules*, 27, 7316-7328 (1994).

Park, S.Y., and Franses, E.I., "Hexadecanol Microstructures of Crystallites in Aqueous Dispersions and of Langmuir-Blodgett Monolayers," *Langmuir*, 11, 2187-2194 (1995).

Chang, C.-H., and Franses, E.I., "Adsorption Dynamics of Surfactants at the Air/Water Interface: A Critical Review of Mathematical Models, Data, and Mechanisms," *Colloids and Surfaces A: Physicochemical and Engineering Aspects* (in press) 1995.

Park, S.Y., Peck, S.C., Chang, C.-H., and Franses, E.I., "The Roles of Dispersed Surfactant Particles on the Dynamic Tension Behavior of Aqueous Surfactant Systems," in *Dynamic Properties of Interfaces and Association Structures*, Shah, D., editor, American Oil Chemists Society Press, (in press) 1995.

Sutandar, P., Ahn, D.J., and Franses, E.I., "Microstructure and Water Transport in Spin-Cast Films of Poly(hexylmethacrylate Azobenzene Sulfone), *Thin Solid Films* (in press) 1995.

Franses, E.I., Siddiqui, F.A., Ahn, D.J., Chang, C.-H., and Wang, N.-H.L., "Thermodynamically Consistent Equilibrium Isotherms for Mixtures of Different-Size Molecules, *Langmuir* (in press) 1995.

Invited Lectures

"Equilibrium and Dynamic Adsorption/Tension of Soluble Surfactants at the Air/Water Interface: A Survey of Models, Data, and Mechanisms," ACS Local Section Meeting, Cincinnati, OH, March, 1995.

"Adsorption and Tension Behavior of Surfactants, Lipids, and Proteins at the Air/Water Interface: Engineering vs. Chemistry," Procter and Gamble Company, Cincinnati, OH, March, 1995.

"Surfactants and Interfacial Phenomena at thze Air/Water Interface," Abbott Laboratories, North Chicago, IL, April, 1995.

"Pulsating-Bubble Tension Measurements and Mathematical Models of Aqueous Surfactants and Lipids," International Workshop "Bubble and Drop 1995," Empoli, Italy, May, 1995.

Meeting Presentations

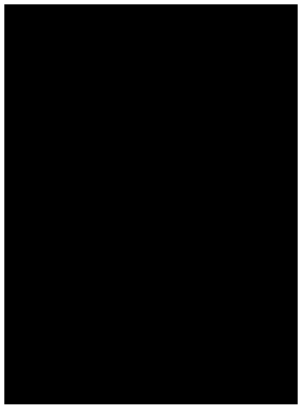
Dynamic Surface Tension Behavior of Aqueous Hexadecanol and Hexadecanol/DPPC Dispersions: The Roles of Dispersed Surfactant Particles and Adsorption Hysteresis," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Pulsating-Bubble Tension Measurements: Data, Method Analysis, and Mathematical Models," AIChE Annual Meeting, San Francisco, CA, November, 1994.

Robert A. Greenkorn

1965

Professor 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

Equilibrium thermodynamics

System modeling

Awards and Major Appointments

Advisory Board of *Journal of Chemical and Engineering Data.*

Editorial Board of *Transport in Porous Media.*

Member of the Board of Directors, Midwest Universities.

Consortium for International Activities (MUCIA).

Member of the University Corporation for Atmospheric Research (UCAR).

Research Coordinator for the Indiana Pollution Prevention Institute.

Research Areas

Group Contribution Thermodynamics and Phase Equilibria of Polar Fluids: The goal of this research is to develop mathematical models and computational methods for the determination of the phase transition properties of polyatomic fluids via computer simulation. To facilitate phase equilibria computations involving dense liquid states, a new algorithm based on temperature perturbation has been developed. This temperature perturbation method does not rely on particle insertions, which are difficult at high densities. For square-well and Lennard-Jones fluids, good agreement has been found between the free energies calculated with our method and other results in the literature.

Fractal Modeling of Mixing in Heterogeneous Porous Media: Currently we are running computer controlled dispersion experiments in order to obtain more detailed length versus dispersivity data. The data collected will allow us to test the hypothesis that a fractal model can be used to explain and predict the apparent increase of dispersivity as the scale of observation increases. A simple numerical model of dispersion matched homogeneous and heterogeneous results generated using the computer. Non-local theory is being tested with the experimental data.

Publications

Sternberg, S.P.K. and R.A. Greenkorn, "An Experimental Investigation of Dispersion in Layered Heterogeneous Porous Media," *Transport in Porous Media, 15*, 15-30 (1994).

Watson, B.S., R.A. Greenkorn, and K.C. Chao, "Molecular Simulations of Metastable, Spinodal, Binodal and Critical States," *Proc. Int. Symp. on Thermodynamics in Chemical Engineering and Industry*, Beijing (1994).

Jin, Z., R.A. Greenkorn, and K.C. Chao, "Correlation of Vapor-Liquid Equilibrium Ratio of Hydrogen, *AIChE Journal* (in press) 1995.

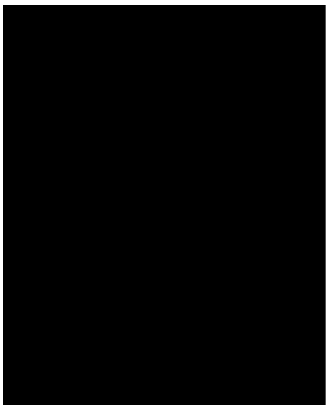
Meeting Presentations

Perkins, M.M., J.H. Cushman, and R.A. Greenkorn, "An Examination of a Stochastic Nonlocal Theory for Modeling Dispersion on Scale Dependent Porous Media," International Conference on Mathematical Modeling of Flow in Porous Media," St. Etienne, France, May, 1995.

Robert E. Hannemann

1969

Visiting Professor



Interests

Aerosols in medical practice

Surfactants in respiratory distress syndrome treatment

Non-invasive diagnostic techniques

Serum bilirubin determination by skin reflectance

Awards and Major Appointments

Medical Technology Committee — Indiana Corporation for Sciences and Technology.

Purdue Engineering Alumni Association — Board of Directors.

Research Areas

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

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

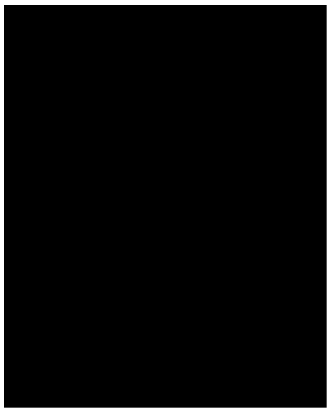
Non-invasive diagnostic techniques: This research is also in the preliminary investigative phase. The goal is to focus the expertise of the various engineering disciplines on the area of non-invasive techniques. The initial effort is the use of skin reflectance measurements to measure serum bilirubin levels, particularly in newborn infants. A second project is the use of sonic technologies to detect and quantify various physiologic measurements. This research is being done in conjunction with Professor George Wodicka (Electrical Engineering).

Serum bilirubin determination by skin reflectance: This work is being done in conjunction with Professor David DeWitt (Mechanical Engineering). Current goal is to develop previous research information into a commercial product.

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

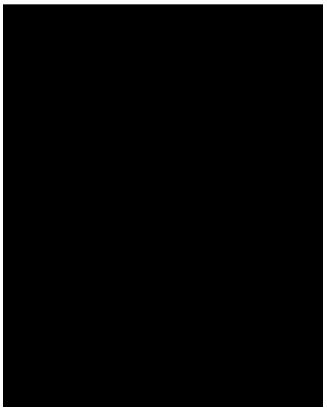
Chairman of *Awards Committee*, Cooperative Education Division, American Society for Engineering Education.

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

Publications

"Drying of Shrinking Biological Materials," with Achanta, S., Okos, M., and Cushman, J., *Proceedings of ISOPOW Practicum - II: Food Preservation by Moisture Control*, Universidad de las Americas - Puebla, Mexico (in press) 1994.

"Moisture Transport in Shrinking Biopolymers During Drying," with Achanta, S., Okos, M., and Cushman, J., *AIChEJ* (submitted).

Basics of Momentum, Heat, and Mass Transfer, with Greenkorn, R., to be published by Academic Press.

Meeting Presentations

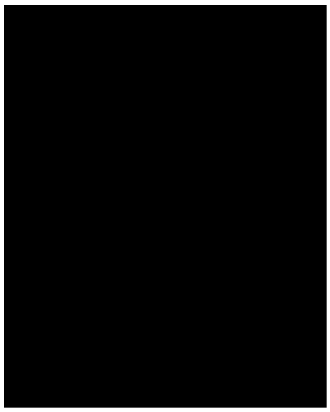
"Moisture Mobility in Shrinking Biological Materials" with Achanta, S., Okos, M., and Cushman, J., American Institute of Chemical Engineers Annual Meeting, San Franciso, CA, November, 1994.

Hilary S. Lackritz

(formerly Hilary L. Hampsch)

1991

Assistant Professor



Degrees

BS, Northwestern University, 1985

PhD, Northwestern University (Materials Science and Engineering), 1990

Interests

Nonlinear Optics

Polymer Physics and Local Dynamics

Optical and Electrical Properties of Polymers

Polymer Surfaces and Interfaces

Awards and Major Appointments

Presidential Faculty Fellows Award (NSF) (1993-1998).

Office of Naval Research Young Investigator Award (1992-1995).

American Physical Society (Division of High Polymer Physics) Publications Committee (1993-).

Research Areas

Research Areas: Polymer physics of electro-optic polymers for photonic devices: A new class of polymeric nonlinear optical (NLO) materials is being developed that utilizes the electro-optic effect. Doped and side- and main-chain functionalized poly(methyl methacrylates), polyphenylenes, indoles, and other novel polymers and polymer blends are being examined. To properly develop and study these second order NLO materials an understanding of the processing-related issues regarding the conductivity in ultrathin films, including charge transport and mobility, and the relationship between the electrical and nonlinear optical properties of the material must be achieved. Electric fields effects are studied using electrochromism, dielectric relaxation, conductivity, optics, and spectroscopy. Monte-Carlo simulations are also used to characterize charge transport effects in these materials. Studying the optical and electrical effects in these materials creates a sensitive method for studying local properties in polymers as a function of processing structure. Devices will be fabricated to show feasibility and studies of compatibility with fiber optics and microelectronics packaging processing will be performed.

Persistence length of local motion in polymers during processing: Basic experimental and theoretical study is being done comparing the relationship between the observed nonlinear optical behavior of polymers upon thermal and mechanical processing to that observed with traditional methods including mechanical and dielectric techniques.

Local or small scale properties are examined using second harmonic generation and solid state nuclear magnetic resonance spectroscopy. Bulk properties are studied using techniques including dynamic mechanical analysis, dielectric relaxation, and differential scanning calorimetry. Doped and side- and main-chain functionalized polymers with identical nonlinear optical chromophores are used to compare rotational mobilities of chromophores located in different parts of the polymer structure. The local mobility is examined in order to determine which parts of the polymer chain participate in a given motion; in particular the motion required to orient the chromophore in response to an applied field is examined. A model based on rotational Brownian dynamics has been developed to describe the chromophore orientation during and following processing.

Structure/Property Relationships and Polymer Physics in High Temperature Polymers for Second Order Nonlinear Optics: Because of the nonequilibrium nature of the glassy state, polymer micro-structures and properties change with time below the glass transition temperature. Therefore, it is critically important to understand the physics of these systems so that one can better predict the long-term behavior and changes in properties throughout their anticipated service life when used for engineering applications. We study structure/property relationships and polymer physics, specifically microviscoelastic and mechanical relaxations as a function of thermal and temporal processing, using nonlinear optics and traditional characterization methods in high temperature stable polymers for second order nonlinear optical applications. A mathematical model with some predictive capabilities that describes the rotational Brownian motion of chromophores in a polymer matrix is developed to simulate the thermal, temporal, and field-dependent behavior. The electric field effects (including residual surface voltage, field-induced bulk charges, and thermally injected charges) can therefore be deconvoluted from the chromophore Brownian motion to reveal information concerning local mobility in polymers. A first ever attempt is made to determine the contributions of the residual surface voltage, field-induced bulk charges, and thermally injected charges to the rotational motion of the chromophores. Experimental verification is obtained using second order nonlinear optics and dielectric relaxation. This study is expected to give a better understanding of the complex kinetic properties below the glass transition, which will be necessary in predicting and controlling the second order nonlinearity for practical applications.

Processing considerations for gas phase polymerization of thermally and environmentally stable optical quality polymers onto metallic substrates: This research concerns the characterization of "gas phase" photopolymerization of vinyl monomers onto metallic substrates as a function of processing conditions. Solvent-free, "gas phase" photopolymerization shows promise in creating defect-free, uniform thin films with excellent electrical and optical properties for commercial applications such as protective coatings and electrical insulators. Other techniques for making thin films, such as Langmuir-Blodgett deposition and spin-coating, yield films that have poor physical properties, are inhomogeneous, or are difficult to make. The issues to be considered in this proposal are how the final film quality is related to the interface and the polymerization mechanism and kinetics, and the characterization of the gas phase reactions. As a part of my long-term

goal to design novel nonlinear optical techniques to study polymer processing, we will develop surface second harmonic generation to characterize the dynamics at the metal/polymer interface. By using surface second harmonic generation (SSHG), issues that have not been resolvable in the past, including reaction rate laws and the dependence of the film properties on interfacial characteristics, can be effectively examined in a continuous, real-time manner. This research has two important deliverables: i) the development of an improved, generally applicable, analytical nonlinear optical technique for studying reactions at surfaces in real time, and ii) the resolution of important processing and characterization issues in a technologically useful polymerization method.

Publications

Wright, M. E.; Mullick, S.; Lackritz, H. S.; Liu, L.-Y. "Organic NLO Polymers. 2. A Study of Main Chain and Guest-Host $c^{(2)}$ NLO Polymers: NLO-phore Structure Versus Poling," *Macromolecules*, *27*, 3009 (1994).

Wright, M.E.; Toplikar, E.G.; Lackritz, H.S.; Kerney, J.T. "Organometallic NLO Polymers 4. Organometallic Main-Chain, Side-Chain, and Guest-Host Polymers: A Study of Their Orientation and Relaxation Using Second Harmonic Generation," *Macromolecules, 27*, 3016 (1994).

Liu, L. Y.; Ramkrishna, D.; Lackritz, H. S. "Rotational Brownian Motion of Chromophores and Electric Field Effects in Polymer Films for Second Order Nonlinear Optics," *Macromolecules, 27*, 5987 (1994).

Lackritz, H.S.; Liu, L.-Y.;Wright, M.E.; Mullick, S. "Study of Poling and Relaxation in Kink and Linear Main-Chain Functionalized Polymers for Second Order Nonlinear Optical Applications," *Macromolecules, 28*, 1912 (1995).

Fu, C.-Y. S.; Lackritz, H. S.; Priddy, D. B.; McGrath, J. E. "Synthesis and Characterization of High Temperature Stable Polymers for Second Order Nonlinear Optical Applications," *Materials Research Society Symposium Series, 328*, 589 (1994).

Priddy, D. B.; Fu, C.-Y. S.; Lackritz, H. S.; McGrath, J. E. "Phosphorus Containing Poly(arylene ether)s as Second Order Nonlinear Optical Materials," *Materials Research Society Symposium Series, 328*, 547 (1994).

Haber, K. S.; Ostrowski, M. H.; Lackritz, H. S. "Characterizing the Distribution of Space Charge in Poled Polymer Films," *Materials Research Society Symposium Series, 328*, 595 (1994).

Wright, M. E.; McFarland, I.; Pettys, B. J.; Lackritz, H. S.; Liu, L. Y. "Organic NLO Polymers. 5. Homopolymerization of Indole Based NLO-phore: A Heterocycle $c^{(2)}$ Main-Chain Polymer," *Polymer Preprints*, *35(1)*, 470 (1994).

Lackritz, H. S.; Ostrowski, M. H.; Liu, L.-Y.; Fu, C.Y. S.; "Dielectric Relaxation and Electric Field Effects in Polymers For Second Order Nonlinear Applications," *Polym. Mater. Sci. Eng. Preprints, 70*, 392 (1994).

Subramanyan, S.; Chen, F.; Lackritz, H. S. "Nonlinear Optical Studies of Photopolymerization at the Metal Interface," *Polymer Preprints*, *35(2)*, 277 (1994).

Lackritz, H. S.; Liu, L.-Y. "Polymer Relaxations in Polymers for Second Order Nonlinear Optical Applications," *Polymer Preprints*, *35(2)*, 202 (1994).

Wright, M. E.; McFarland, I.; Lackritz, H. S.; Subramanyan, S.; Liu, L. Y. "A Novel Approach for the Synthesis of Side-Chain, IPN, and Cross-linked Nonlinear Optical Polymers," *Polymer Preprints*, *35(2)*, 126 (1994).

Fu, C.Y.-S; Priddy, D. B.; McGrath, J. E.; Lackritz, H. S. "Polymer Physics for Second-Order Nonlinear Optics," *Proc. Soc. Photo-Opt. Instrum. Eng.*, *2258*, 153 (1994).

Pasmore, T.; Talbot, J.; Lackritz, H. S. "Monte-Carlo Simulations of Electric Field Hopping in Doped Polymer Thin Films," *Nonlinear Optics* (in press) to appear in June, 1995.

Wright, M. E.; Toplikar, E. G.; Lackritz, H. S.; Subramanyan, S. "A Preliminary Study of Poly(p-phenylene) Based NLO Materials," *Chem. Mater.* (in press).

Wright, M. E.; Toplikar, E. G.; Lackritz, H. S.; Kerney, J. T. "New Organometallic Polymeric Materials: The Search for Organometallic NLO Polymers," in *Inorganic and Organometallic Polymers*, Alcock, H., Wynne, K., and Wisian-Neilson, P., Eds., ACS Symposium Series #XXX, American Chemical Society, Washington, D.C. (in press).

Chen, F.; Subramanyan, S.; Lackritz, H.S. "Photopolymerization Dynamics of Acrolein onto Metal Substrates Using Surface Second Harmonic Generation," *Materials Research Society Symposium Series* (in press).

Sullivan, L. A.; Lackritz, H. S. "Dynamic Mechanical Analysis and Dielectric Relaxation for Second Order Nonlinear Optical Applications," *Materials Research Society Symposium Series* (in press).

Invited Lectures

"Polymer Relaxations in Doped and Functionalized Systems Studied Using Second Order Nonlinear Optics," Society for Photo-optic Instrumentation Engineers, San Diego, CA, July, 1994.

"Polymer Physics in Poled Polymers Studied Using Second Order Nonlinear Optics, Dielectric Relaxation, and Dynamic Mechanical Analysis," Wright-Patterson Air Force Base, Dayton, OH, August, 1994.

"Polymer Relaxations in Doped and Functionalized Systems Studied Using Second Order Nonlinear Optics," American Chemical Society/ Optical Society of American, Washington, DC, August, 1994.

"Polymer Physics and Electric Field Effects in Poled Polymers for Second Order Nonlinear Optical Applications," Cornell University, Department of Chemical Engineering, Ithaca, NY, September, 1994.

"Processing of Polymers for Second Order Nonlinear Optics," Engineering Research Center, University of Wisconsin, Madison, WI, October, 1994.

"Design and Development of Polymers for Second Order Nonlinear Optics," Utah State University, Department of Chemistry, Logan, UT, December, 1994.

"Polymer Physics Studied Using Second Order Nonlinear Optics," University of Nebraska, Department of Mechanical and Materials Engineering, Lincoln, NE, February, 1995.

"Characteristic Relaxation Times in Polymers Studied by Nonlinear Optics, Dielectric Relaxation, and Dynamic Mechanical Analysis," Wright-Patterson Air Force Base, Dayton, OH, April, 1995.

"Polymer Physics Studied Using Second Order Nonlinear Optics," Massachusetts Institute of Technology, Polymer Seminar Series, Cambridge, MA, May, 1995.

Chaired Conferences/ Symposia

Session Chair and Organizer- "Polymers for Optoelectronics and Photonics," American Institute of Chemical Engineers Meeting, San Francisco, CA, November, 1994.

Session Chair- "Electrically and Optically Active Polymers II," American Physical Society Meeting, San Jose, CA, March, 1995.

American Chemical Society/Optical Society of America (ACS/OSA) Symposium on Thin Films for Photonic Applications (member International Advisory Committee 1994-).

ACS Program Chair 1995 Portland OSA meeting.

Symposium Organizer 1998 Orlando ACS meeting.

Meeting Presentations

"Nonlinear Optical Studies of Photopolymerization at the Metal Interface," American Chemical Society/Optical Society of American national meeting, Washington, DC, August, 1994.

"Second Harmonic Generation and Dielectric Relaxation Studies of High Temperature Nonlinear Optical Polymers," American Institute of Chemical Engineers national meeting, San Francisco, CA, November, 1994.

"The Rotational Brownian Motion of Chromophores and Electric Field Effects in Polymer Films for Second Order Nonlinear Optics," American Institute of Chemical Engineers national meeting, San Francisco, CA, November, 1994.

"Electric Field Effects in Polymer Thin Films Studied Using Electrochromism, Dielectric Relaxation and Second Order Nonlinear Optics," American Physical Society national meeting, San Jose, CA, March, 1995.

"Electro-optic and Second Harmonic Generation Studies of Dye-Doped Thin Film Polymers," American Physical Society national meeting, San Jose, CA, March, 1995.

"Kinetic Studies of Photopolymerization at Metal Surfaces Using Surface Second Harmonic Generation," American Physical Society national meeting, San Jose, CA, March, 1995.

"Charge Transport through Chromophore Doped Polymer Thin Films for Second Order Nonlinear Optics," American Physical Society national meeting, San Jose, CA, March, 1995.

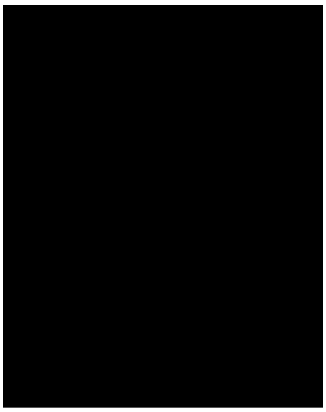
"Dynamic Mechanical Analysis and Dielectric Relaxation for Electro-Optical Polymer Applications," Materials Research Society national meeting, San Francisco, CA, April, 1995.

"Gas Phase Photopolymerization of Vinyl Monomers on Metallic Substrates Studied Using Surface Second Harmonic Generation," Materials Research Society national meeting, San Francisco, CA, April, 1995.

Joseph F. Pekny

1990

Associate Professor



Degrees

BS, Princeton University, 1985

PhD, Carnegie-Mellon University, 1989

Interests

Process scheduling, planning, and design

Parallel and distributed computing

Simulation

Combinatorial optimization

Nonlinear optimization

Software engineering methods

Research Areas

Distributed and Parallel Solution of Large Scale Linear Programs: The amount of detail addressed by combinatorial optimization methods is directly proportional to the size of linear programs that can be routinely solved. Indeed, the type of formulation, exact algorithm, or heuristic used to solve problems all implicitly depend on the number of variables and constraints which can be solved using a given amount of time. In the worst case, lack of sufficient linear program solution capability can preclude the use of formal solution methods, dramatically decreasing the probability of effectively solving a combinatorial optimization problem over a nontrivial set of instances. Thus, increasing the amount of engineering and business detail that can be addressed in applications critically depends on expanding the size of linear programs that can be solved in a branch and bound context. With respect to the Distributed Control Architecture for Branch and Bound (DCABB) system developed within our group over the last few years, accelerated solution time of linear programs will remove the root node of the branch and bound search tree as a bottleneck to computation. Currently, DCABB is effective at distributing branch and bound computations among multiple machines once tree search commences but operates in a sequential mode during solution of the root node. Successful development of a distributed method for solving linear programs will allow DCABB to be enhanced to process the root node in a distributed fashion. Thus, computational resources will be effectively employed for the entire duration of calculations. Given the effectiveness of DCABB in many applications, the root node is now a significant portion of the overall wall clock time. Perhaps more important, distributed solution of linear programs offers the potential for shared storage of constraint information with the net effect that avail-

able fast memory can be the sum of the memory available on the network. Currently, the size of a linear program is limited to that which can be stored in the machine on the network with the most memory. Therefore, addressing memory considerations is important to routinely piercing the one hundred thousand to one million constraint barrier. Ultimately, no single machine involved in a DCABB computation will possess all of the linear programming information necessary to conducting branch and bound. Successfully implementing distributed solution of linear programs will require a means of overcoming the latencies inherent in network computations. Undoubtedly, this is the most significant conceptual barrier to distributed linear program solution, although issues of work load balancing, network robustness, and scalability will also have to be simultaneously addressed to produce an effective approach.

The starting point for the distributed linear programming project has been the LP++ system which is an object-oriented solver constructed in C++ to serve as a foundation for DCABB. LP++ was developed within our research group and so the source code and sequential expertise is available as a foundation. However, the key to effectively distributing calculations is not simply devising a distribution scheme for the classic simplex method or existing interior point methods. Rather, the key is to explore automating decomposition schemes (e.g. Dantzig-Wolfe decomposition) that dualize key constraints into the objective function and result in linear programming subproblems that can be solved independently. Once the subproblems are solved, the dualized constraint multipliers can be updated. Iteration continues until the multipliers are optimal and the overall linear program is solved. Intuitively, decomposition based approaches can be thought of as a hybrid of direct methods (e.g. simplex) and iterative methods that update connecting constraint multipliers. Fortunately, most large linear programs resulting from engineering applications naturally decompose on the basis of problem physics making the proposed approach plausible. This research project necessarily investigates multiplier updating in a distributed context, automated means for decomposing problems, and scalability issues for up to several hundred processors. The scalability issues are nontrivial since the number of distributed subproblems is typically larger than the number of subblocks in the constraint matrix (e.g. the number of plants in a planning application).

The most effective parallelization strategies are often hierarchical in nature. Thus, underneath the decomposition layer, lower level parallelization opportunities are being investigated to take advantage of multiple processors that might be available on a given machine in a network. These lower level opportunities include, in order of granularity: (i) pursuit of multiple optimization paths on or inside polyhedron implied by a problem, (ii) parallel linear algebra, and, for simplex based approaches, (iii) simultaneous pivoting and pricing. Although parallelization at these levels is certainly not scalable to a large number of processors, in a hierarchical scheme these layers can result in O(10) speedup at each layer with up to 50% processor efficiency. Research will also be conducted as to the appropriate distribution of processors across the decomposition and lower level parallelization layers for a massively parallel machine where latency is at least an order of magnitude smaller than in a distributed environment.

Rigorous Methods for Practical Process Scheduling and Planning: The business climate of the 1990s and beyond is characterized by intense international competition, strong cost cutting pressures, environmental regulation, and globalization. Chemical process industry success in such a climate requires effective scheduling and planning to efficiently use capacity and to quickly adapt to changes in the marketplace. A large number of constraints, the increasing scope of operations, time and efficiency pressures, and the combinatorial complexity implied by discrete decisions make scheduling and planning problems difficult to solve. This research project is laying the foundation for a new generation of process scheduling and planning tools that are based on rigorous optimization methods, yet are robust to failure, flexible, easy to use in an industrial environment, can be quickly integrated with corporate databases, and can address very large and highly constrained scheduling and planning problems. An important attribute of using rigorous optimization methods is that, in the worst case, they provide an estimate of the best achievable performance available and, in the best case, they produce a schedule or plan that is provably optimal for a given industrial scenario. In a competitive environment, estimates of absolute operating efficiency are critical to the process of continuous improvement that are the basis for corporate survival. The key philosophy of this research project is to provide the methodology and information necessary for understanding and controlling the critical components of process performance in a system that is sufficiently flexible to incorporate technology advances and that is designed to account for the fact that the scheduling and planning function will continue to evolve over time.

This research project is intended to address a number of challenges uncovered by our previous work and specifically accomplish the following objectives: (i) development of a formulation specifically tuned to sequencing considerations that will complement existing formulations and be able to address a range of processes in considerable detail, (ii) development of an efficient means to strengthen the formulation of scheduling problems through the introduction of strong inequalities derived from problem physics, (iii) development of large scale integer programming solution capability specific to scheduling and planning problems and sufficient to address long time scales, and (iv) integration of symbolic reasoning and mathematical programming methods to dramatically reduce the training required to use a sophisticated system and mitigate the robustness problems inherent in exclusive use of rigorous methods on combinatorial optimization problems. This research project will also contribute to the advancement of knowledge concerning the solution of more general integer programming problems in that much of the proposed methodology will transfer to other problem domains. Given that a significant portion of the research is experimental in nature, the infrastructure resulting from it will represent a significant resource base from which to pursue a variety of other engineering decision problems.

Process Re-engineering, Retrofit, and Design Under Uncertainty: With respect to short term process management, process re-engineering, retrofit, and design involve several additional considerations including (i) long time horizon, (ii) multiple geographically distributed facilities, (iii) transportation costs, (iv) uncertainty in market conditions and productive capacity, and (v) corporate strategy. Of course a

new process or any changes to an existing process must be consistent with low level operating details, otherwise the process structure cannot be implemented or are not sufficiently ambitious. Theoretically, a comprehensive detailed model could be built and used as the basis for determining process structure, but such a model would be impossibly large to solve for almost every application. Practically, such a model is unnecessary since detailed operating projections several weeks, months, or years into the future will certainly not be implemented as they are projected because of changes in conditions. As an alternative to a monolithic detailed model, we propose developing hierarchical models that divide the time axis over the horizon of interest into a number of segments. An aggregate Mixed Integer Linear Programming (MILP) model taking into account resource constraints, production capacity, demands, possible equipment types, costs, and material balances is then built using such a non-uniform discretization of time. For a one year horizon, there may be twenty-five time segments. The actual number of time segments is controlled by the size of the aggregate model and the available computational resources to be applied to solving it. Within each time segment, the aggregate model is applied recursively if the time segment is long or a detailed problem is solved to determine if the production assignments of the aggregate model can be met if the time segment is short. If a detailed model determines that the aggregate model requires too much production, information is fed back to the aggregate model in the form of constraints which further limit production allocation within the time segment. Subsequent solution of the aggregate model will then require more realistic production targets and can adjust production over the entire horizon accordingly. Thus our approach ultimately produces a number of detailed problems that are coordinated by the aggregate model. In a batch context, these detailed production problems can be addressed using our scheduling technology. In a continuous context, they can be addressed with commercial simulators.

Market or process uncertainty can be incorporated by making parameters random variables and imposing an objective function that seeks to accommodate uncertainty, e.g. maximize expected net present value. Unfortunately, such direct treatment greatly complicates solution efforts by introducing severe nonlinearity. With current solution technology and foreseeable computational capability, such nonlinearity greatly compromises the size of problems that can be addressed and eliminates possible consideration of many practical issues. As an alternative to such direct treatment of uncertainty, we have developed the concept of scenarios. Intuitively, a scenario is a set of estimates of demand for products during a given time segment along with an associated probability. In a given time segment, the sum of scenario probabilities must be one. A user is free to specify scenarios in different time segments independently. Continuous probability distributions can be approximated by using scenarios and the quality of approximation scales with the total number of scenarios. Computational expense also scales with the number of scenarios but the aggregate model remains an MILP. The objective function of the aggregate model can reflect direct economic considerations (e.g. minimize expense, maximize expected net present value, etc.) or product-based objectives (e.g. plan to meet the most probable demands for products).

To summarize, this project involves addressing the following issues for long term management implied by process re-engineering, retrofit, and design: (i) segmentation of time, (ii) lumping of production elements, (iii) handling uncertainty through the concept of scenarios, and (iv) a rigorous mechanism for feeding information back from the subproblems to the aggregate model. Once these issues are resolved, the approach will be capable of addressing worldwide business applications on a routine basis with users retaining control over strategic issues and the model determining the implications of implementing strategy in an uncertain environment.

Publications

Pekny, J.F. and D.L. Miller, "A Staged Primal-Dual Algorithm for Finding a Minimum Cost Perfect Two-Matching in an Undirected Graph," *ORSA Journal on Computing*, Vol. 6, No. 1, pp. 68-81 (1994).

Gooding, W. B., J. F. Pekny, and P. S. McCroskey, "Enumerative Approaches to Parallel Flowshop Scheduling via Problem Transformation," *Computers and Chemical Engineering*, Vol. 18, No. 10, pp. 909-927 (1994).

Subrahmanyam, S., J. F. Pekny, and G. V. Reklaitis, "Design of Batch Chemical Plants Under Uncertainty," *Industrial and Engineering Chemistry Research*, 33, pp. 2688-2701 (1994).

Zentner, M. G., J. F. Pekny, G. V. Reklaitis, and J. N. D. Gupta, "Practical Considerations in Using Model Based Optimization for the Scheduling and Planning of Batch/Semicontinuous Processes," *Journal of Process Control,* Vol. 4, No. 4, pp. 259-280 (1994).

Kudva, G. and J. F. Pekny, "DCABB: A Distributed Control Architecture for Branch and Bound Calculations," *Computers and Chemical Engineering*, Vol. 19, No. 6/7, pp. 847-865 (1995).

Miller, D. L. and J. F. Pekny, "A Staged Primal-Dual Algorithm for Perfect b-Matching With Edge Capacities," *ORSA Journal on Computing* (in press).

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Meeting Presentations

"The Role of High Speed Networks in Distributed Branch and Bound Calculations," High Speed Network Jamboree, San Diego, CA, 1994.

"Combinatorial Optimization in Engineering Systems: Exploiting Problem Structure and Parallelism," Proceedings of the 1993 NSF Design and Manufacturing Systems Conference, Massachusetts Institute of Technology, 1994.

"Perspectives on Model Based Integration of Process Operations," Proceedings of the Fifth International Symposium on Process Systems Engineering, Kyjongu, Korea, 1994.

Using Distributed Computing to Support Integrated Batch Process Scheduling, Planning, and Design Under Market Uncertainty," Foundations of Computer Aided Process Design 94, Snowmass, CO, poster session, 1994.

"A Branch-and-Cut Algorithm for Vehicle Routing Problems," ORSA/TIMS meeting, Detroit, MI, Fall 1994.

"Designing, Retrofitting, and Planning for a Globally Integrated Chemical Business," ORSA/TIMS meeting, Detroit, MI, Fall 1994.

"Special Purpose Linear Programming Relaxation Algorithms," ORSA/TIMS meeting, Detroit, MI, Fall 1994.

"A Support System for Planning and Scheduling Global Process Operations," ORSA/TIMS meeting, Detroit, MI, Fall 1994.

"A Hierarchical Model for Batch Process Design Under Uncertainty," ORSA/TIMS meeting, Detroit, MI, Fall 1994.

"A Mathematical Programming Approach to the Energy Minimization of Model Proteins," AIChE Fall National Meeting, session 62, poster session, San Francisco, CA, 1994.

"Distributed Solution of Large Scale Mixed Integer Programs with Application to Batch Plant Design and Scheduling," AIChE Fall National Meeting, session 223, San Francisco, CA, 1994.

"A Framework for Global Planning, Design, and Decision Making in the Batch Processing Industry," AIChE Fall National Meeting, session 225, San Francisco, CA, 1994.

"Polyhedral Relationships Between Different Representations of Optimization Problems" AIChE Fall National Meeting, session 233, San Francisco, CA, 1994.

"A Heuristic for Constrained Cutting Stock Problems," AIChE Fall National Meeting, session 235, San Francisco, CA, 1994.

"A Hierarchical Decomposition Approach to Planning and Scheduling of Batch Production Facilities Under Market Uncertainty," AIChE Spring National Meeting, Houston, TX, 1995.

"A Hierarchy for Integrated Process Simulation, Scheduling, and Design/Retrofit Tools," Simulation MultiConference, The Society for Computer Simulation, Phoenix AZ, 1995.

"Techniques for Problem Size Reduction in the Design of Large Scale Batch Chemical Plants Under Market Uncertainty," European Symposium on Computer Aided Process Engineering-5, Bled, Slovenia, 1995.

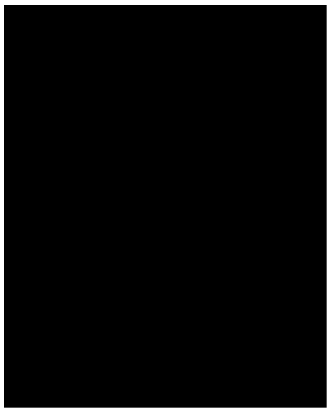
"Combinatorial Optimization in Engineering Systems: The Role of High Performance Computer Networks," Computer Science Department, Carnegie Mellon University, Pittsburgh, PA, August, 1994.

"Towards the Convergence of the Computing/Communication Revolution, Engineering Systems, and Combinatorial Optimization," Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA, 16th Annual Graduate Student Research Symposium, Keynote Speaker, October, 1994.

Nicholas A. Peppas

1976

Showalter Distinguished Professor of Chemical and 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

APV Medal, International Pharmaceutical Association (1995).

Best Paper Award, Annual Meeting American Institute of Chemical Engineers (1994).

Best Session Award, Annual Meeting American Institute of Chemical Engineers (1994).

Award and Honorary Membership, Italian Society of Medicine and Natural Sciences (1994).

Food, Pharmaceutical and Bioengineering Award, American Institute of Chemical Engineers (1994).

Research Areas

Diffusion in and Dissolution of Glassy Polymers: Penetrant transport in glassy polymers is 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. Experimental studies are performed with well-characterized samples of polystyrene and poly(methyl methacrylate) in various solvents using laser interferometry 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.

Multifunctional Polymerization Kinetics and Network Structure: The mathematical modeling of multifunctional polymerization/crosslinking reaction 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, changes in the kinetics of these polymerizations are studied. The conversion-time profiles are obtained at different light intensities using a calorimetric and a spectroscopic technique.

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 is 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 homopolymer. 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.

Drug and Protein Transport in and Interactions with Porous and Non-porous Biohydrogels: Drug and protein transport in porous and non-porous hydrogels is investigated in an effort to identify the main structural parameters that affect solute diffusion in such systems. Well

characterized polymer and copolymer samples of crosslinked poly(acrylic acid) are prepared and their molecular structure is analyzed in terms of molecular weight between crosslinks, mesh size, equilibrium degree of swelling and degree of ionization. The nature of the swelling agent is expressed by its pH, ionic strength and concentration. Drug/polymer interactions are quantified with a modified ATR/FTIR technique. By preparing porous and non-porous forms of these hydrogels we are able to study the influence of the porous structure on solute transport. These studies contribute to a variety of fields including bioseparations, biosensor development and controlled release.

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. Upon loading these systems with drugs or proteins and upon abruptly changing the pH of the surrounding solution from acidic to basic, it is possible to decomplex the network leading to sudden drug release. An alternative release system based on interprenetrating 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.

Solute Delivery Using Ionic Systems: The delivery of drugs, peptides and proteins in medical or biological applications under oscillatory conditions can be achieved by utilizing ionic hydrogels. Such polymers respond to changes in pH or ionic strength by expanding or contracting. A range of porous and non-porous cationic polymer networks will be prepared and their dynamic swelling and equilibrium characteristics will be investigated. Drugs and proteins are incorporated and their time-dependent, relaxation controlled, pH-dependent behavior is investigated. These studies will be used to develop better systems for biosensors, bioseparations and controlled release.

New Bioadhesive Polymers for Targeting: The effect of crosslinking, polymer hydrophilicity, and interdiffusion on the adhesion and cohesion of bioadhesive hydrogels in contact with mucin will be investigated. Hydrogels are prepared by free radical polymerization of acrylic acid, 2-hydroxy ethyl methacrylate and ethylene glycol dimethacrylate. The surface chemistry of selected polymers is modified by grafting poly(ethylene glycol) of varying molecular weight. 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.

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am Ende, M.T. and N.A. Peppas, "Analysis of Drug Distribution in Hydrogels Using FTIR Microscopy," *Pharm. Res.*, (in press).

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am Ende, M.T., D. Hariharan and N.A. Peppas, "Factors Influencing Drug and Protein Transport and Release from Ionic Hydrogels," *Reactive Polymers*, (in press).

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Tissue Engineering (1994-).

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

European Journal of Pharmaceutics and Biopharmaceutics, (1992-).

Invited Lectures

"Probing the Nature of the Mucoadhesive Behavior of PEG and PAA-Containing Hydrogels via ATR-FTIR Spectroscopy, Near Field FTIR Spectroscopy and the Falling Liquid Film Technique," Cygnus Therapeutic Systems, Redwood City, CA, September 15, 1994.

"Trends, New Technologies and Smart Polymers in Controlled Release," Colorcon, Princeton, NJ, October 12, 1994.

"Issues in Contemporary Hydrogels Research for Medical Applications," University of Wisconsin, Department of Chemical Engineering, Madison, WI, December 1, 1994.

"Chain Interpenetration and Fracture in Gel/Gel and Gel/Mucin Adhesion," Michigan State University, Department of Chemical Engineering, East Lansing, MI, February 16, 1995.

"Bioadhesive Poly(vinyl alcohol) as a Carrier for Controlled Release of Proteins and Factors for Wound Healing," Sankyo Company, Research Institute, Tokyo, Japan, March 7, 1995.

"Smart Materials in Medicine Applications," Ventritex Co., Sunnyvale, CA, April 5, 1995.

"Contemporary Hydrogels Research," Kagoshima University, Department of Applied Chemistry and Chemical Engineering, Kagoshima, Japan, April 17, 1995.

Chaired Conferences/ Symposia

Chairman of Session on "Drug Delivery," 11th Congress of the International Society for Artificial Cells, Blood Substitutes and Immobilization Biotechnology," Boston, MA, July, 1994.

Chairman of Session on "Hydrogels," Society for Biomaterials Meeting, San Francisco, CA, March, 1995.

Organizer and Chairman of Symposium on "Polymer/Inorganic Interfaces," Materials Research Society Meeting, San Francisco, CA, April, 1995.

Chairman of Session on "Biomedical Polymers," Kagoshima, Japan, April, 1995.

Chairman of Session on "Microparticles," World Conference on Pharmaceutical Technology, Budapest, Hungary, May, 1995.

Meeting Presentations

"Recent Advances in Mucoadhesives for Drug Delivery," 11th Congress of ISABI, Boston, MA, July 25, 1994.

"Crosslinking Methods: Applications to Controlled Release," Fourth Workshop on Controlled Delivery in Consumer Products, Chicago, IL, September 27, 1994.

"Past, Present and Future of Materials in Medicine," Meeting of Society of Medicine and Natural Sciences, Parma, Italy, October 3, 1994.

"Future Directions in the Development of Biomaterials," Annual Meeting of the Biomedical Engineering Society, Tempe, AZ, October 15, 1994.

"Mechanochemical Behavior of pH- and Temperature-Sensitive Gels," Annual Meeting of the Biomedical Engineering Society, Tempe, AZ, October 16, 1994.

"Measurement of Chain Interpenetration at a Mucoadhesive Interface Using ATR-IR Spectroscopy," First Iranian Chemical Engineering Conference, Teheran, Iran, November 15, 1994.

"Intelligent Biomaterials: Scientific Curiosity or Panacea?," Annual AIChE Meeting, San Francisco, CA, November 15, 1994.

"P(NIPAAm-co-MAA) Hydrogels for Temperature-and pH-Sensitive Release of Antithrombotic Agents," Annual AIChE Meeting, San Francisco, CA, November 15, 1994*e*.

"P(NIPAAm-co-MAA) Hydrogels for Temperature- and pH-Sensitive Release of Antithrombotic Agents," Annual AIChE Meeting, San Francisco, CA, November 16, 1994.

"Mechanistic Aspects and Transport Behavior during Polymer Dissolution," Annual AIChE Meeting, San Francisco, CA, November 14, 1994.

"Understanding of Dissolution of Semicrystalline Polymers," Annual AIChE Meeting, San Francisco, CA, November 14, 1994.

"Evidence of Mucoadhesion by Chain Interpenetration at a PAA/Mucin Interface Using ATR-FTIR Spectroscopy," Annual AIChE Meeting, San Francisco, CA, November 14, 1994, (A)*.

"Adhesive and Diffusive Characteristics of Novel PVA Films for Medical Applications," Annual AIChE Meeting, San Francisco, CA, November 15, 1994.

"Kinetics of Multifunctional Acrylates for Information Storage Systems," Annual AIChE Meeting, San Francisco, CA, November 15, 1994.

"Semicrystalline Polymers for Controlled Drug Delivery," Indianapolis/Cincinnati Meeting, AAPS, Indianapolis, IN, February 16, 1995.

"Release of Antithrombotic Agents," Indianapolis/Cincinnati Meeting, AAPS, Indianapolis, IN, February 16, 1995.

"New Interpolymer Complexes, Star Polymers and Ionic Hydrogels in Drug Delivery Applications," Seventh International Symposium on Recent Advances in Drug Delivery Systems, Salt Lake City, UT, February 28, 1995.

"Pulsatile Release of Antithrombotic Agents from pH- and Temperature Sensitive Hydrogels," Seventh International Symposium on Recent Advances in Drug Delivery Systems, Salt Lake City, UT, February 28, 1995.

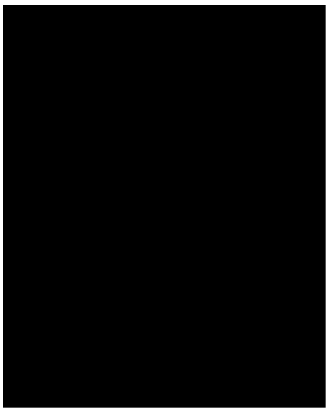
"Polymer Dissolution: A Modeling Attempt to "Couch" Molecular Theories in a Phenomenological Framework," American Physical Society Meeting, San Jose, CA, March 22, 1995.

"Recent Advances in Modeling and Physicochemical Behavior of Swellable Polymers, Biomaterials, and Drug Delivery Systems," 5th Iketani Conference and International Symposium on Biomedical Polymers, Kagoshima, Japan, April 19, 1995.

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

Melchor Visiting Professor, University of Notre Dame (Fall 1994).

Visiting Professor, Institute for Advanced Studies in Biological Process Technology (May 8 - June 3, 1994).

Visiting Professor, Jawaharlal Nehru Centre for Advanced Scientific Research (June 13 - Aug. 8, 1994).

UDCT Diamond (Distinguished Alumnus Award, Bombay University) (August, 1994).

Research Areas

Chemical Reaction Engineering: The emphasis here is on pattern formation in catalytic reactors in which the catalyst phase is coaxed to form spatial and temporal patterns as a means to promote product selectivity in multi-reaction systems. Methods of nonlinear mathematics are brought to bear on heterogeneous models to develop concepts of stability of a continuous class of steady states in a packed bed reactor. Spatial patterns can be induced in packed bed reactors by introducing multiple feeds as a start-up strategy. Stability of pattern *classes* which assure product quality is under investigation.

Dispersed Phase Systems: Our research focuses on the fundamental processes of coalescence and redispersion generated by hydrodynamic forces in liquid-liquid dispersions. Past effort through inverse problem methodologies on dynamic drop size distribution data has resulted in quantitative understanding of drop break-up and coalescence rates in turbulent dispersions as a function of drop size, dispersed phase fraction and surface charge. Recent thrust is on controlling drop size by manipulating drop size distributions for improving selective yields of desired products over wasteful by-products in reaction systems.

In such systems, while conventional wisdom calls for small drops to increase reaction rates, selectivity is often promoted by large droplets. Coalescence processes are being investigated in food emulsions as a function of various additives with the objective of promoting shelf-life of food products. Our recent work shows that destabilization of food emulsions occurs not as much by coalescence of drops in the bulk as by coalescence in a dense cream layer.

Biochemical Engineering: Cybernetic models have been developed which can describe contrasting situations of sequential as well as simultaneous uptake of mixed, substitutable substrates accounting for dependence on preculturing of the organisms. The models have also been shown to describe growth dual-limiting complementary substrates in batch, fed-batch and continuous cultures. Nonlinear mathematical analysis revealing the models' full stability structure which governs microbial response to complex media is under way. Cybernetic models are found to be ideally suited to probe problems in biodegradation of aromatic hydrocarbon pollutants in view of their potential to generate bioremediation strategies towards maximizing degradation of pollutants. A specific example is the manipulation of bacterial metabolism with different co-metabolites to maximize growth rate as well as the rate of biodegradation. On another front, a self-similar theory of microbial populations has been advanced to make quantitative interpretations about processes in single cells from dynamic population data obtained from flow cytometers.

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. With Professor Caruthers, our effort has been in the development of efficient stochastic methods for the conformation of polymer molecules in the presence of an external field. Also in progress is modeling of the glassy state of polymers using stochastic models on mesoscopic scale.

Publications

Straight, J.V. and D. Ramkrishna, "Cybernetic Modeling and Regulation of Metabolic Pathways. Application to Growth on Complementary Substrates," *Biotech. Progress, 10*, 574-587 (1994).

Straight, J.V. and D. Ramkrishna, "Cybernetic Modeling and Regulation of Metabolic Pathways. Application to Growth under Multiply-Limiting Conditions," *Biotech. Progress, 10*, 588-605 (1994).

Trinh, S. and D. Ramkrishna, "Feasibility of Pattern Formation in Catalytic Reactors," *Chem. Eng. Sci, Vol. 49(1),* 158-1599 (1994).

Manjunath, S., K.S. Gandhi, R. Kumar and D. Ramkrishna, "Precipitation in Small Systems - I. Stochastic Analysis," *Chem. Eng. Sci., Vol. 49(9)*, 1451-1463 (1994).

Wright, H. and D. Ramkrishna, "Factors Affecting Coalescence Frequency of Droplets in Stirred Liquid-Liquid Dispersion," *A.I.Ch.E. J., Vol. 40(5)*, 676-686 (1994).

Ramkrishna, D., "Toward a Self-Similar Theory of Microbial Populations," *Biotech. & Bioeng.*, *43*, 138-148 (1994).

Liu, Lee-Yin, D. Ramkrishna, and H. Lackritz, "The Rotational Brownian Motion of Chromophores and Electric Field Effects in Polymer Films for Second Order Nonlinear Optics," *Macromolecules*, 21, 5987-5999 (1994).

Ramkrishna, D. and A. Sathyagal, "Analysis of Dispersed Phase Systems. Fresh Perspective," *AIChE J., 41(1)*, 35-44 (1995).

Sathyagal, A., D. Ramkrishna, and G. Narsimhan, "Solution of Inverse Problems in Population Balances. II. Particle Break-up," *Computers and Chem. Eng., 19*, 437-451 (1995).

Sathyagal, A., G. Narsimhan, and D. Ramkrishna, "Breakage Functions of Droplets in a Stirred Liquid-Liquid Dispersion from Experimental Drop Size Distributions," *Chem. Eng. Sci.* (in press).

Kumar, S. and D. Ramkrishna, "On the Solution of Population Balance Equations by Discretization I," *Chem. Eng. Sci.* (in press).

Kumar, S. and D. Ramkrishna, "On the Solution of Population Balance Equations by Discretization II," *Chem. Eng. Sci.* (in press).

Ramkrishna, D. and K. Yasuda, "Maximizing Selectivity of Liquid-Liquid Reaction Systems. Control of the Dispersion Process," *Chem. Engi. Commns. (*submitted).

Manjunath, S., K.S. Gandhi, R. Kumar, and D. Ramkrishna, "Precipitation in Small Systems - II, *Chem. Eng. Sci.* (submitted).

Gandhi, K.S., R. Kumar, and D. Ramkrishna, "Some Basic Aspects of Reaction Engineering of Precipitation Processes," *Ind. & Eng. Chem.* (submitted).

Ramakrishna, R., D. Ramkrishna and A. E. Konopka, "Cybernetic Modeling of Growth in Mixed, Substitutable Substrate Cultures. Sequential and Preferential Utilization," *Biotech. & Bioeng.* (submitted).

Trinh, S. and D. Ramkrishna, "Pattern Formation in Fixed Bed Catalytic Reactors - I," *Chem. Eng. Sci.* (submitted).

Lam, A., A. Sathyagal, S. Kumar and D. Ramkrishna, "On the Maximum Stable Drop Diameter in Stirred Dispersions," *A.I.Ch.E. J* (submitted).

Invited Lectures

"Inverse Problems in Population Balances" in Conference on Advances in Chemical Engineering, Indian Institute of Chemical Technology, Hyderabad, India, August 9-11, 1994.

"A Self-Similar Theory of Microbial Population Growth," Department of Chemical Engineering, Indian Institute of Science, Bangalore, India, August 3, 1994.

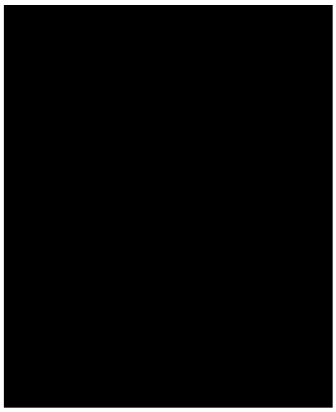
"Population Balances," Department of Chemical Engineering, University of Notre Dame, December, 1994.

"Strategies for Enhancement of Bioremediation from Cybernetic Modeling of Mixed Substrate Utilization," Biochemical Engineering IX, Engineering Foundation Conference, Davos, Switzerland, May 21-26, 1995. In the session on "The Role of Physiology for Process Enhancement," May 23, 1995.

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

Fellow, AIChE.

ASEE Chemical Engineering Division Lectureship Award (1994).

Computers & Chemical Engineering, Pergamon Press/Elsevier Science, Editor in Chief.

Computer Applications in Engineering Education, Editorial Board.

Council for Chemical Research, Member, Governing Board (1994-1997).

Kirkpatrick Chemical Engineering Achievement Award, Board of Judges, Chair (1995).

Publications

Tsirukis, A.G., and G.V. Reklaitis, "Application of Generalized Hopfield Networks to Discrete Nonlinear Optimization Problems," *Computers & Chem. Engng.*, *18*, 459-468 (1994).

Kanakamedala, K., G.V. Reklaitis and V. Venkatasubramanian, "Reactive Schedule Modifications in Multipurpose Batch Chemical Plants," *Ind. Eng. Chem. Res*., *33*, 77-90 (1994).

Kudva, G., A. Elkamel, J.F. Pekny and G.V. Reklaitis, "A Heuristic Algorithm for Scheduling Multiproduct Plants with Production Deadlines, Intermediate Storage Limitations, and Equipment Changeover Costs," *Computers & Chem. Engng., 18*, 859-876 (1994).

Jayakumar, S., and G.V. Reklaitis, "Chemical Plant Layout Via Graph Partitioning Part I, Single Level," *Computers & Chem. Engng., 18,* 441-458 (1994).

Subrahmanyam, S., J.F. Pekny, and G.V. Reklaitis, "Design of Batch Chemical Plants under Market Uncertainty," *Ind. Eng. Chem., Res.* 33, 2688-2701 (1994).

Zentner, M.G., J.F. Pekny, G.V.Reklaitis and J.N.D. Gupta, "Practical Considerations in Using Model Based Optimization for the Scheduling and Planning of Batch/Semicontinuous Processes," *Journal of Process Control*, special issue on Batch Processing, 5, No.4, 259-280 (1994).

Yi, G. and G.V. Reklaitis, "Model-Based Feedback Inventory Controller for Intermediate Storage in Batch Processes," *J. Process Control*, special issue on Batch Processing, 5, No. 4 , 227-237 (1994).

Jayakumar, S., R.G. Squires, G.V.Reklaitis, P.K. Andersen, B.C. Choi, and K.R. Graziani, "The Use of Computer Simulations in Engineering Capstone Courses: a Chemical Engineering Example—The Mobil Catalytic Reforming Process Simulation, "*Int. J. Engr. Educ.*, 9, 243-250 (1994).

Androulakis, I. and G.V. Reklaitis, "Analysis of the Spurious Behavior of Asynchronous Relaxation Algorithms," *Computers & Chem. Engng.*, 19, 827-845 (1995).

Yi, G. and G.V. Reklaitis, "Reducing the Effects of Failure Propagation in Periodic Processes involving Intermediate Storage with Multiple Input/Multiple Output Streams," *Korean J. of Chem. Eng.*, 12, 123-131 (1995).

Jayakumar, S., R.G. Squires, G.V. Reklaitis, and K.S. Grassi, "Simulating the Air Products Cryogenic Hydrogen Reactive Cooling Process," *Chem. Eng. Ed.*, 29, 26-31 (1995).

Davis, J.M., G.E. Blau, and G.V. Reklaitis, "Computers in Undergraduate Chemical Engineering Education: A Perspective on Training and Application," *Chem. Eng. Ed.*, 29, 26-31 (1995).

Reklaitis, G.V., "Computer-Aided Design and Operation of Batch Processes," *Chem. Eng. Ed.*, 29, 76-85 (1995) (Text of Award Lecture).

Lee, B. and G.V. Reklaitis, "Optimal Scheduling of Batch Processes for Heat Integration: I: Basic Formulations," *Computers & Chem. Engng.*, 19, 867-882 (1995).

Lee, B. and G.V. Reklaitis, "Optimal Scheduling of Batch Process for Heat Integration: II: Extended Problems," *Computers & Chem. Engng.*, 19, 883-906 (1995).

Jayakumar, S. and G.V.Reklaitis, "Chemical Plant Layout via Graph Partitioning, Part II: Multiple Levels," *Computers & Chem. Engng.* (in press).

Zentner, M.G., A. Elkamel, J.F. Pekny, and G.V. Reklaitis, "A Language for Describing Process Scheduling Problems," *Computers & Chem. Engng.*, Rippin Memorial Issue (in press).

Bassett, M.H., F.J. Doyle III, G.K. Kudva, J.F. Pekny, G.V. Reklaitis, S. Subrahmanyam, M.G.Zentner, and D.L. Miller, "Perspectives on Model Based Integration of Process Operations," *Comput. Chem. Engng*, special issue, Selected Papers from PSE'94 (in press).

Jayakumar, S., R.G. Squires, G.V.Reklaitis, P.K. Andersen, and B.K. Dietrich, "The Purdue-Dow Styrene Butadiene Polymerization Simulation," *Int. J. Eng. Educ.* (in press).

Reklaitis, G.V., "Overview of Scheduling and Planning of Batch Process Operations," in *Batch Processing Systems Engineering*, Reklaitis, Rippin, Hortacsu and Sunol (eds), Springer Verlag, NATO ASI Series F, 1995 (in press).

Reklaitis, G.V., "Future Directions for R&D in Batch Process Engineering," in *Batch Processing Systems Engineering*, Reklaitis, Rippin, Hortacsu and Sunol (eds), Springer Verlag, NATO ASI Series F, 1995 (in press).

Papageorgaki, S., A.G. Tsirukis and G.V. Rekaitis, "The Influence of Resource Constraints on the Retrofit Design of Multipurpose Batch Chemical Plants," in *Batch Processing Systems Engineering*, Reklaitis, Rippin, Hortacsu and Sunol (eds), Springer Verlag, NATO ASI Series F, 1995 (in press).

Zentner, M.G., and G.V. Reklaitis, "An Exact MILP Formulation for the Scheduling of Resource Constrained Batch Chemical Processes," in *Batch Processing Systems Engineering*, Reklaitis, Rippin, Hortacsu and Sunol (eds), Springer Verlag, NATO ASI Series F, 1995 (in press).

Mockus, L., and G.V. Reklaitis, "A New Global Optimization Algorithm for Batch Process Scheduling," *Proc. State of the Art in Global Optimization: Computational Methods and Applications,* Princeton, NJ (in press).

Invited Lectures

"The Role of Simulation and Optimization in Batch Process Design & Operations," Dow Chemical Research Center, Midland, MI, December, 1994.

"Scheduling Approaches for the Batch Process Industries," World Batch Forum, PA, May 22-24, 1995.

"A Language for Describing Process Scheduling Problems," D.W.T. Rippin Memorial Session, 5th European Symposium on Computer Aided Process Engineering, Bled, Slovenia, June 13, 1995.

Chaired Confences/ Symposia

Fourth International Conference on Foundations of Computer Aided Process Design, Advisory Committee member and Contributed Papers chair, Snowmass, CO., July 10-15, 1994.

International Organization for Process Systems Engineering, Executive Committee member, 1988-present.

Meeting Presentations

"A Framework for Global Planning, Design, and Decision

Making in the Batch Processing Industry," paper 225b, AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Asynchronous Distributed Decision Making with Applications to Process Operations Problems," paper 233n, AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Mathematical Programming Formulation for Scheduling of Batch Operations using Nonuniform Time Discretization," paper 235d, AIChE Annual Meeting, San Francisco, CA, November, 1994.

"A New Global Optimization Algorithm for Batch Process Scheduling," Symposium on State of the Art in Global Optimization" Princeton, NJ, April, 1995.

"Techniques for Problem Size Reduction in the Design of Large Scale Batch Chemical Plants under Market Uncertainty," 5th European Symposium on Computer Aided Process Engineering (ESCAPE 5), Bled, Slovenia, June 11-14, 1995.

"Mathematical Programming Formulation for Scheduling of Batch Operations based on Nonuniform Time Discretization," 5th European Symposium on Computer Aided Process Engineering (ESCAPE 5), Bled, Slovenia, June 11-14, 1995.

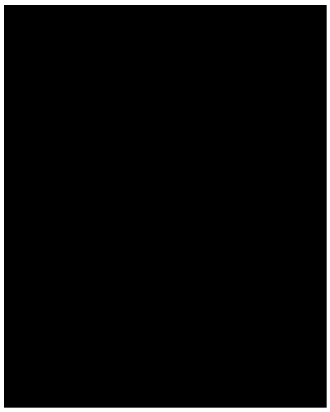
"Issues in Solving Large Scale Planning, Design, and Scheduling Problems in Batch Chemical Plants," 5th European Symposium on Computer Aided Process Engineering (ESCAPE 5), Bled, Slovenia, June 11-14, 1995.

"A Framework for Investigating Schedule Robustness under Uncertainty," 5th European Symposium on Computer Aided Process Engineering (ESCAPE 5), Bled, Slovenia, June 11-14, 1995.

Eva Sevick-Muraca

1994

Assistant Professor



Degrees

Ph.D, Carnegie Mellon University, 1989

M.S, University of Pittsburgh, 1985

B.S, magna cum laude, University of Pittsburgh, 1983

Interests

Biomedical optical diagnostics

Biomedical optical imaging

Process monitoring and control using measurements of photon migration

Optical measurements of particle size and polydispersity

Awards and Honors

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

National Science Foundation Young Investigator, (1993-1998).

Whitaker Foundation Biomedical Research Awardee, (1991-1994).

National Institutes of Health Postdoctoral Research Fellow, (1989-1991).

Research Areas

The following is a synopsis of the research projects ongoing in the Photon Migration Laboratory at Purdue University, School of Chemical Engineering: **Measurements of photon migration for tissue diagnostics:** Recent advances in laser diode technology and photodetection make possible the development of non-invasive, near-infrared tissue diagnostics as an economic alternative to more costly diagnostic clinical tests. Current near-infrared technologies are based upon measuring the attenuation of light as it passes through tissues. Unfortunately, the intense and variable scattering properties of tissue prevent quantitative diagnostics from the amount of light transmitted. In our research, instead of measuring the amount of light transmitted through tissues, we measure its migration characteristics. Specifically, we measure the distribution of picosecond photon "time-of-flights" for photons transmitted across several centimeters of tissues. From such measurements, we employ the diffusion approximation to describe the transport of light in random media to quantitate scattering and absorption parameters. From parameter estimates of absorption, we have shown the capacity for non-invasive determination of brain tissue oxygenation for such crucial procedures as coronary bypass and cardiac transplant. In addition, we are developing measurement of photon migration for measurement of tumor oxygenation in order to

assist oncologists in the efficacious choice and staging of therapeutic interventions. We continue to develop photon migration instrumentation, measurement, and data analysis for non-invasive and economical quantitation of tissue physiology and pathophysiology.

Photon migration imaging for breast cancer screening: In recent years, the early detection of preclinical breast cancer in screening programs has been proposed and implemented as a beneficial tool against a disease which one in nine women will experience in the United States. While current breast cancer screening programs implement conventional x-ray mammography and palpation for breast cancer detection, there are recognized limitations to x-ray mammography. Generally, conventional x-ray mammography is not used for early premenopausal women due to the increased cellularity and subsequent radiodense tissue structure. The benefit achieved from x-ray mammography screening in this population outweighs the small yet finite risk associated with repeated doses of x-irradiation. Yet when compared to postmenopausal women who significantly benefit from x-ray mammography, premenopausal women with preclinical breast cancer may experience more rapid tumor growth because of hormone fluctuations. This suggests not only the need for more frequent screening in this population, but more importantly, an alternative means of cancer detection which is not compromised by the increased tissue cellularity found in early premenopausal women.

In our research program, we have developed a biomedical optical imaging device which is dependent upon the radiative scatter for image formation. The new imaging technique, called Photon Migration Imaging (PMI), is not compromised by tissue scatter, but is enhanced by it. Essentially, the new technology consists of illuminating a tissue with light whose intensity is sinusoidally modulated at MHz frequencies. The light which is re-emitted is both phase-shifted and demodulated with respect to the incident light. We have demonstrated that rapidly acquired phase-shift and modulation "images" contain direct information for detection and localization of 1-3 mm size heterogeneities obscured by tissue-like scattering. In our studies, we focus upon tissue phantom studies and computational models in which the presence of diseased tissues or other optical heterogeneities can be imaged and detected in near real time. It is anticipated that the resulting studies will not only provide a foundation for future clinical trials of PMI breast cancer screening in patients who are not candidates for conventional mammography, but will also help establish a new imaging modality for industrial applications.

Lifetime-based spectroscopy in tissues and other random media: The development of stable and non-toxic near-infrared (NIR) optical probes promises non-invasive, diagnostic spectroscopy for tissues and other random media. However, studies show that quantitative determination of (bio-) chemical composition from re-emitted fluorescence spectra requires deconvolution of scattering and absorption properties. Since tissue optical properties can be expected to vary from person to person and with pathophysiology, it is unlikely that fluorescence intensity measurements will make use of the emerging NIR optical probes. Likewise, since chemical sensing in process streams often involve streams with variable scatter densities, fluorescence intensity measurements will require tedious calibration for quantitative monitoring.

In this research project, we have coupled established techniques of frequency-domain measurements of optical probe lifetimes together with a simple algorithm for excitation and fluorescent light propagation in tissues in order to quantitate metabolite and other chemical species concentrations. The lifetime-based approach differs from intensity measurements in that calibration is not necessary and deconvolution of tissue optical properties is not required. However, for short-lived optical probes (~ ps and ns lifetimes), photon migration times must be accounted for accurate determination of probe lifetime. Using computational approaches which account for photon migration, we have shown that photon migration times are readily accounted for by simple "referencing" measurements. We have also discovered that long-lived optical probes cannot probe beyond the sub-surfaces of tissues and other random media when non-invasive measurements are employed. This is a crucial finding since the development of luminescent and phosphorescent probes for non-invasive tissue pO_2 measurements is currently progressing in industry without the proper understanding of the role of photon migration plays in defining the origin of such signals.

These coupled studies of photon migration and fluorescence/phosphorescence kinetics are imperative for the successful development of NIR optical probes as diagnostic tools in biology, medicine, and process monitoring.

Process monitoring with measurements of photon migration: The measurement of critical variables for chemical and pharmaceutical processes involving polymer melts, powders, polydisperse slurries, and high solid contents is often limited to time-consuming, off-line laboratory analyses. Consequently, the control schemes for continuous production in many of these processes cannot be implemented and end product quality is ultimately the variable upon which process conditions are set. On-line spectroscopic measurements provide an efficient and versatile measurement of critical variables necessary for process control. However, their predictiveness is destroyed by the radiative scatterer in such process streams.

In this set of projects, we are developing novel measurements of photon migration to investigate the optical characteristics of a process stream to give quantitative, and rapid, online information of:

(i) absorption by chemical species,
(ii) mean hydrodynamic particle size,
(iii) scatterer density, and
(iv) polydispersity.

Measurement of photon migration provides a self-calibrating measure of the *transport* characteristics of light rather than the *amount* of light detected. Consequently, these measurements are not subject to the limitations which occur in attenuation measurements. In one project sponsored by industry, we are currently developing a prototype photon migration instrument for on-line process monitoring of TiO_2 polydispersity in a high solid content process stream. We are also assessing the potential for quantitation of chemical composition via multi-wavelength measurements and lifetime-based optical probes.

Major Appointments

Beckman Laser Institute and Medical Clinic Biotechnology Resource Advisory Committee, University of California, Irvine, (January, 1995-).

Editorial Advisory Committee, Optical Society of America, Biomedical Optics Journal (October, 1994-).

National Institutes of Health Review Panel, Special Study Section, (1993-).

Measurement and Control Engineering Center, University of Tennessee (Knoxville), National Science Foundation Industrial/University Cooperative Research Center, (September, 1993-).

Computer Integrated Process Operations Consortium, School of Chemical Engineering, Purdue University, (May, 1995-).

National Science Foundation I/UCRC for Industrial Pharmacy, Purdue University, (May, 1995-).

Publications

Sevick, E.M., J.K. Frisoli, C.L. Burch, and J.R. Lakowicz, "Localization of absorbers using frequency-domain measurements of time-dependent photon migration," Applied Optics, 33, 3562-3570 (1994).

Sevick-Muraca, E.M. and C.L. Burch "The origin of phosphorescent and fluorescent signals in tissues," *Opt. Lett., 19*, 1928-1930 (1994).

Burch, C.L., and J.R. Lakowicz, and E.M. Sevick-Muraca, "Fluorescence lifetime based sensing in tissues: a computational study," *Biophys. J., 68,* 1574-1582 (1995).

Sevick, E.M. "Computations of time-dependent photon migration for biomedical optical imaging," In: *Methods in Enzymology, Numerical Computer Methods, Part B*., Volume 240, L. Brand and M. Johnson, (Eds.), Academic Press; Orlando, FL. pp. 748-781, *(invited)* 1994.

Sevick, E.M., C.L. Burch, J.K. Frisoli, M.L. Johnson, K. Nowaczyk, H. Szmacinski, and J.R. Lakowicz. "The physical basis of photon migration imaging using frequency-domain measurements," *Medical Optical Tomography: Functional Imaging and Monitoring*, I. Müller, (Ed.) Proc. Soc. Photo-Opt. Instrum. Eng., Optical Engineering Press, Bellingham, WA, pp. 485-512, *(invited)* 1994.

Chaired Conferences/ Symposia

"Advances in Laser and Light Spectroscopy to Diagnose Cancer and other Diseases II" Biomedical Optics Meeting, The International Society for Optical Engineering, San Jose, CA, February, 1995.

"Optical tomography, photon migration, and spectroscopy of tissue and model media: theory, human studies, and instrumentation," Biomedical Optics Meeting, The International Society for Optical Engineering, San Jose, CA, February, 1995.

"Lasers in Medicine and Science," Conference of Lasers and Electro-Optics, Optical Society of America, Baltimore, MD, May, 1995.

Invited Lectures

"Photon migration measurements for biomedical optical spectroscopy and imaging," Eastern Analytical Conference, New York, NY, November 17, 1994.

"Measurement of photon migration using frequency-domain tech-

niques for optical spectroscopy and imaging in random media," Ontario Laser and Lightwave Research Center, Toronto, March 7, 1995.

"The basics of photon migration spectroscopy," Mallinckrodt Medical, St. Louis, MO, April 18, 1995.

"Measurements of photon migration in optically dense particulate suspensions," Pacific Northwest Laboratories, Richland, WA, March 10, 1995.

"Measurements of photon migration for non-invasive optical diagnostics and imaging," American Society for Laser Medicine and Surgery, San Jose, CA, April 2, 1995.

Meeting Presentations

"Optical property measurements and propagation of light in tissues," Biomedical Engineering Society Annual Meeting, Tempe, AZ, October, 1994.

"Determination of fluorescent lifetimes from non-invasive measurements of phase-shift: a computational study," Biomedical Engineering Society Annual Meeting, Tempe, AZ, October, 1994.

"Dynamic measurement of photon migration for particle sizing in optically dense suspensions," American Institute of Chemical Engineers, November, 1994.

"The feasibility of photon migration for breast cancer screening," Biomedical Optics Conference, Society of Photo-Instrum. Eng., February, 1995.

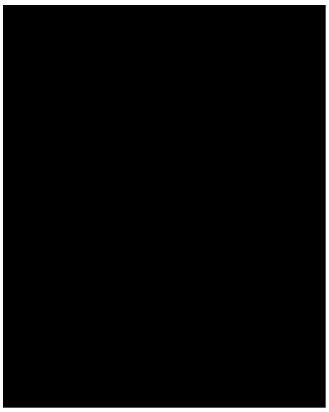
"The origin of phosphorescent and fluorescent signals re-emitted from tissues,"American Society for Laser Medicine and Surgery, San Diego, CA, 1995.

"Fluorescence spectroscopy and imaging in tissues," Conference of Lasers and Electro-optics, Baltimore, MD, May, 1995.

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

Awards and Major Appointments

CMA National Catalyst Award for Outstanding Teaching (1995).

ASEE Chester F. Carlson Award for Engineering Teaching (1995).

Publications

S. Jayakumar, R.G. Squires, G.V. Reklaitis, P.K. Andersen, B.C. Choi and K.R. Graziani, "The Use of Computer Simulations in Engineering Capstone Courses: A Chemical Engineering Example - The Mobil Catalytic Reforming Process Simulation," *Int. J. Engr. Educ.*, 9 (3), 243-250 (1994).

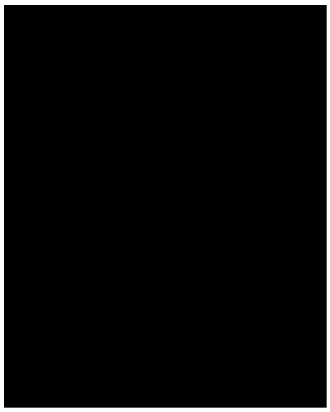
S. Jayakumar, R.G. Squires, G.V. Reklaitis, P.K. Andersen, and B.K. Dietrich, "The Purdue-Dow Styrene-Butadiene Polymerization Simulation," *J. Eng. Educ.*, (in press) 1995.

S. Jayakumar, R.G. Squires, G.V. Reklaitis, K.S. Grassi, "Simulating the Air Products Cyrogenic Hydrogen Reactive Cooling Process," *Chem. Eng. Educ*., Vol. 29, No. 1, pp. 26-31 (1995).

Christos G. Takoudis

1981

Associate Professor



Degrees

DEng, National Technical University, Athens, 1977

PhD, University of Minnesota, 1982

Interests

Microelectronic Materials and Processing

Heteroepitaxy in Group IV Semiconductors

In Situ Surface Enhanced Raman Spectroscopy and FTIR at Interfaces

Heterogeneous Catalysis

Reaction Engineering

Awards and Major Appointments

Member of the Editorial Board of the Journal: *Chaos, Solitons and Fractals - Applications in Science and Engineering*

Research Areas

Microelectronic Materials and Processing: Major problems related to semiconductor materials and processing include answers to questions like: (i) Can we obtain impurity-free substrate surfaces before processing steps? (ii) How does the growth of single crystalline thin films take place in chemical vapor deposition (CVD) systems? What are the key surface chemical phenomena during these processes? (iii) What are the contributions of gas phase reactions to the growth and structure of single crystalline microelectronic films? (iv) Can we control the composition, structure and properties of such thin films through changes in the processing environments? (v) Can we develop new materials? (vi) Can we control the growth of thin films on patterned substrates so that the properties of microelectronic films grown on seed windows of different sizes are uniform (e.g., seed window size-independent)? (vii) Can we predict, analyze and possibly eliminate masking film degradation phenomena during surface cleaning techniques of patterned substrates? (viii) Can we model chemical vapor deposition processes so that given any processing environment we could predict the properties of the thin films to be grown? Or given the desired properties of thin films to be grown, could we predict the processing environments needed?

Since the basic aspects in CVD systems include coupling among reaction kinetics on substrate surfaces and in the gas phase, transport phenomena, thermodynamics, and reactor modeling, a chemical engineering background would be of critical importance in addressing fundamental questions like the ones mentioned above. In fact, chemical en-

gineers have been increasingly involved in major problems related to microelectronic materials and processing over about the last twelve years. Hence, there has been a fair amount of research on III-V materials (e.g., GaAs being an outstanding example of them), II-VI materials, and other compound semiconductors. Also, there has been some emphasis on dry etching, plasma-enhanced processes, and lithography. Although silicon has been by far the material of choice in the semiconductor industry, basic questions like the ones mentioned above have remained unanswered for silicon as well as other group IV semiconductors (e.g., Si-Ge, SiC). Also, as issues regarding increased overall yields, for example, in the semiconductor industry became critically important, the need for fundamental research on the problems mentioned above became increasingly apparent. Further, optical properties of Si-Ge semiconductors and highly attractive properties of SiC thin films in microelectronics have recently opened up new research opportunities in group IV materials and processing.

In this area, our group's major thrust is relationships among processing, properties and structure as well as the development of new materials. Novel substrate surface cleaning techniques, kinetics and surface chemistry of reaction processes on silicon substrate surfaces, controlled production of thin heterostructure layers, and constrained single crystalline growth of silicon-based heterostructures are novelties of this research.

In our microelectronics research the main thrusts are homoepitaxy in group IV materials and heteroepitaxy in group IV compound and alloy semiconductors. The objective is to design new material systems and methods for fabrication of group IV semiconductors, to enhance the understanding of material properties for use in optical and electronic systems, and to explore novel structures with confined stable SiC, Si and Si-Ge layers. Such work (1) allows exploration of the mechanisms, surface chemistry and kinetics of advanced materials growth, (2) leads to technologically powerful relationships among material behavior, processing environments, optical properties, and defect analyses, and (3) allows production of novel and extremely useful photonic and wide-bandgap structures.

In the design and control of semiconductor manufacturing facilities, our research focuses on a basic understanding of the interactions between unit process selection and design, production control methodologies and facility layout, and on the development of an integrated design methodology for semiconductor fabrication facilities.

Surface Chemistry - Heterogeneous Catalysis: The acquisition of molecular compositional and structural information for adsorbates in heterogeneous catalytic reactions on metal surfaces represents a key step in achieving fundamental understanding of such processes in gas phase environments. The development of the desired *in situ* spectroscopic probes for this purpose provides major challenges, associated primarily with the difficulty of probing the molecularly thin interfacial region without engendering overwhelming spectral interference from the bulk reactor phase. While sample transfer to and from an ultrahigh vacuum environment enables a plethora of "surface science" characterization techniques to be employed, such *ex situ* approaches suffer from an inherently smaller relevance to the catalytic reactor system at hand.

Of the various *in situ* molecular characterization techniques, infrared (IR) spectroscopy has achieved significant success; yet, it is important to recognize several limitations of IR spectroscopy. As a consequence, there remains a crucial need for additional techniques that can yield molecular vibrational information for interfacial species present under genuine catalytic reaction conditions. An interesting, although still remarkably unexplored, alternative technique for this purpose is Raman spectroscopy.

Our group's major thrust in this area is the emergence of a fundamentally new understanding of several key gas phase catalytic processes on metal surfaces over a wide range of temperatures. Time-resolved *in situ* surface-enhanced Raman (SER) spectra of adsorbed species on a subsecond/seconds time scale coupled with reaction rate measurements in transient experiments, including those with isotopic labeling af atoms of interest, have been, are and will result in hitherto unavailable information concerning the nature, role and kinetic significance of reaction intermediates and adsorbed species participating in the mechanisms of the reactions of interest.

In surface chemistry and catalysis, our research focuses on time-resolved *in situ* probing of adsorbed species and reaction intermediates (primarily with Surface-Enhanced Raman Scattering and Infrared Spectroscopy) coupled with *ex situ* spectroscopic techniques (e.g., X-Ray Photoelectron Spectroscopy, Auger Electron Spectroscopy) and reaction rate measurements in transient experiments with or without isotopic labeling of atoms of interest. These studies result in hitherto unavailable information concerning the nature, role and kinetic significance of reaction intermediates and adsorbed species participating in the pathway and mechanism of advanced material growth as well as in heterogeneous catalytic reactions.

Publications

Tolia A.A., R.J. Smiley, W.N. Delgass, C.G. Takoudis and M.J. Weaver, "Surface Oxidation of Rhodium at Ambient Pressures as Probed by Surface-Enhanced Raman and X-Ray Photoelectron Spectroscopies," *J. Catal.*, 150, 56-70 (1994).

Hoffman C.M., E.N. Houstis, J.R. Rice, A.C. Catlin, M. Gaitatzes, S. Weerawarana, N.-H. L. Wang, C.G. Takoudis and D.G. Taylor, "SoftLab - A Virtual Laboratory for Computational Science," *Math. & Comp. in Simulat.*, 36, 479-491 (1994).

Yang S.-K., S. Peter and C.G. Takoudis, "On the Fundamentals of Two Step Etching Techniques for Ideal Silicon-Hydrogen Termination of Silicon(111)," *J. Appl. Phys.*, 76, 4107-4112 (1994).

Lee I.-M. and C.G. Takoudis, "Thermodynamic and Kinetic Studies of $Si_{1-x}Ge_x$ Chemical Vapor Deposition," *Electrochem. Soc.*, 94-1, 623-625 (1994).

Hase R., C.G. Takoudis and R. Uzsoy, "Cellular and Reentrant Layouts for Wafer Fabrication," *ECS Proceedings,* Spring Meeting, 468-470 (1994).

Uzsoy R. and C.G. Takoudis, "Scheduling and Facility Design for Semiconductor Manufacturing," *SEMATECH Operational Modeling Workshop*, Attach. 1-6 (1994).

Panczyk C., and C. G. Takoudis, "*In Situ* FTIR Emission Spectroscopy in Silicon Chemical Vapor Deposition on Si(100) Surfaces," *Proceed. Topical Confer. on Synthesis & Processing of Electronic Materials*, 271-276 (1994).

Hase R., S. Chen, R. Uzsoy and C. G. Takoudis, "Relationships Between Process Fundamentals, Facility Design and Production Control of Semiconductor Manufacturing Systems," *Proceed. Topical Confer. on Synthesis & Processing of Electronic Materials*, 175-180 (1994).

Peter S., S.-K. Yang and C. G. Takoudis, "Fundamental Studies on Chemical Cleaning of Si(100) and Si(111)," *Proceed. Topical Confer. on Synthesis & Processing of Electronic Materials*, 356-361 (1994).

Hase R., C.G. Takoudis and R. Uzsoy, "Cellular and Reentrant Layouts for Semiconductor Wafer Fabrication Facilities," *Proceedings of the International Electronics Manufacturing Technology Symposium*, La Jolla, CA, 112-118 (1994).

Takoudis C.G., G.W. Neudeck and E.P. Kvam, "Interdisciplinary Undergraduate Research in Microelectronic Materials and Processing," *Proceedings of the ASEE Total Quality Education - Illinois/Indiana Sectional Conference*, West Lafayette, IN, 74-77 (1995).

Takoudis C.G., G.W. Neudeck and E.P. Kvam, "Interdisciplinary Undergraduate Research in Microelectronic Materials and Processing," *Proceedings of the University / Government / Industry Microelectronics Symposium*, Austin, TX (in press) 1995.

Kongetira P., G.W. Neudeck and C.G. Takoudis, "Modeling of Selective Epitaxial Growth (SEG) and Epitaxial Lateral Overgrowth (ELO) of Silicon in SiH_2Cl_2-HCl-H_2 System," *Proceedings of the University / Government / Industry Microelectronics Symposium*, Austin, TX (in press) 1995.

Tolia A.A., C.T. Williams, C.G. Takoudis and M.J. Weaver, "Surface-Enhanced Raman Spectroscopy as an In-Situ Real-Time Probe of Catalytic Mechanisms at High Gas Pressures: The CO-NO Reaction on Rhodium," *J. Phys. Chem.* (in press) 1995.

Invited Lectures

"Novel Approaches to Mechanistic Approaches of Catalytic Oxidation on Platinum-Group Transition Metal Surfaces," Annual Meeting, AIChE, San Francisco, CA, November 14, 1994.

"Scheduling and Facility Design for Semiconductor Manufacturing," SEMATECH Operational Modeling Workshop, Austin, TX, October 6, 1994.

"Water Vapor Adsorption on Silicon-Based Substrates," Delco Electronics, Kokomo, IN, May 10, 1995.

"Adsorption-Desorption Phenomena in Silicon-Based Sensors," Delco Electronics, Kokomo, IN, May 18, 1995.

Meeting Presentations

"Reentrant and Cellular Layouts for Silicon Wafer Fab Facilities," Electronics Manufacturing Technology Symposium, La Jolla, CA, September 12-14, 1994.

"*In Situ* FTIR Emission Spectroscopy in Silicon Chemical Vapor Deposition on H-Terminated Si(111) and Si(100) Surfaces," Annual Meeting, AIChE, San Francisco, CA, November 13-18, 1994.

"Relationships Between Process Fundamentals, Facility Design and Production Control of Semiconductor Manufacturing Systems," Annual Meeting, AIChE, San Francisco, CA, November 13-18, 1994.

"On the Fundamentals of Two Step Etching Techniques for Silicon-Hydrogen Termination of Si(111) and Si(100)," Annual Meeting, AIChE, San Francisco, CA, November 13-18, 1994.

"Reaction Path Analysis in Heterogeneous Catalytic Reactors with Real-Time Probing of Adsorbed Reaction Intermediates," Annual Meeting, AIChE, San Francisco, CA, November 13-18, 1994.

"Interdisciplinary Undergraduate Research in Microelectronic Materials and Processing," ASEE Total Quality Education - Illinois/Indiana Sectional Conference, West Lafayette, IN, March 16-18, 1995.

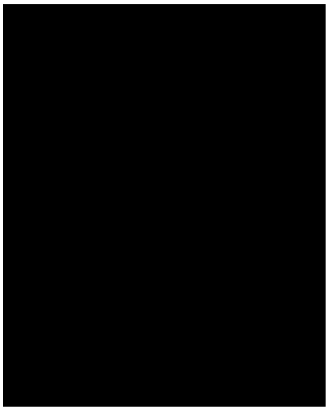
"Interdisciplinary Undergraduate Research in Microelectronic Materials and Processing," University/Government/Industry Microelectronics Symposium, Austin, TX, May 16-17, 1995.

"Modeling of Selective Epitaxial Growth (SEG) and Epitaxial Lateral Overgrowth (ELO) of Silicon in SiH_2Cl_2-HCl-H_2 System," University/Government/Industry Microelectronics Symposium, Austin, TX, May 16-17, 1995.

Julian Talbot

1989

Assistant Professor



Degrees

BA, University of Cambridge, 1981

PhD, Southampton University, 1985

Interests

Statistical mechanics

Computer simulation

Adsorption and interfacial phenomena

Thermodynamic and transport properties of molecular fluids

Nanometer clusters

Awards and Major Appointments

Invited Professor at the Université Pierre et Marie Curie, Paris, France, (1994).

Research Areas

Microscopic theory of protein adsorption phenomena: The adsorption of proteins at the solid-liquid interface is both scientifically intriguing and of great significance in a wide range of applications including biocompatibility, separations and chromatography. Technological advances in these fields depend, wholly or partly, on a fundamental understanding of the adsorption process. In the last few years there has been significant progress towards this goal in response to simultaneous advances in both theory and experiment. At the microscopic level the adsorption is complex involving the transport of the particles from the bulk to the surface region, interactions between the adsorbing particles and those that are already adsorbed, an attachment step, possible changes in the orientation or conformation of the adsorbed molecule (for proteins or polymers), a detachment step and transport away from the surface. As a result of strong interactions between the protein and the solid surface, desorption may be extremely slow causing the adsorption process to appear irreversible on the experimental time scale. As a consequence, one cannot necessarily rely on the methods of equilibrium statistical mechanics, and novel theoretical approaches are required.

Our group has pioneered the development of models for adsorption kinetics that account for non-equilibrium kinetics and the steric hindrance effects at finite coverages. Jeremy Ramsden (Basel) has confirmed the accuracy of the theory in a number of detailed comparisons with experiments for simple proteins such as transferrin and has demonstrated that the kinetic equations are superior to those of the Langmuir model in this application. Other groups, including,

Z. Adamczyk (Cracow), J. Brash (Hamilton), E. Pfefferkorn (Strasbourg), and M. Elimelech (UCLA) are beginning to use our ideas. Adamczyk, for example, has applied the theory to the adsorption of colloid particles.

The theories that we have developed describe accurately the adsorption kinetics of *simple* proteins such as lysozyme and transferrin. In affinity chromatography solutes bind selectively to ligands immobilized on a solid surface. To describe this process we developed the Random Site Model and used it to correlate some experimental breakthrough curves for lysozyme adsorption. The improvement over the Langmuir equation is dramatic, indicating that the new model captures the essential physics, at least for simple proteins. Moreover, the theory yields a unique, self-consistent set of adsorption rate constants. We have also developed equations for the kinetics of multicomponent adsorption based on equilibrium equations of state for mixtures. The predictions of the theory agree well with the results of computer simulations of reversible adsorption processes.

An additional aspect of irreversible adsorption observed experimentally, yet not accounted for in simple models, is the possibility of a particle conformational change following adsorption. Recently, in collaboration with Paul Van Tassel, Gilles Tarjus and Pascal Viot of the Université Pierre et Marie Curie, Paris, we have studied a model which accounts for a surface induced particle conformational change in the form of a change in particle size following adsorption (i.e. spreading). In one dimension, this model is exactly solvable in the case where the spreading is instantaneous. The two dimensional case may be examined via a series expansion in powers of the density. The expansion may be combined with the known asymptotic behavior towards saturation so as to have an approximate description valid over the entire coverage range. The simple formulae which result may be used to investigate the main kinetic features for a wide range of physical parameters, thus facilitating comparison with experimental results.

A full quantitative understanding of the adsorption kinetics also requires that the transport of the particles to the surface be taken into consideration. As part of his PhD thesis, just completed, Ho Suk Choi investigated the influence of various forces, including gravitational, brownian, hydrodynamic and colloidal on the deposition kinetics of spherical particles. For example, to characterize the influence of gravity relative to the brownian force, Ho Suk introduced the dimensionless gravity number and he then studied the deposition process at finite surface coverages with numerical solutions of the convective diffusion equation. We also developed codes to incorporate hydrodynamic interactions between the depositing particles and the surface and preadsorbed particles.

Thermodynamic and transport properties of fluids and fluid mixtures in porous media: The thermodynamic and transport behavior of fluids in confined spaces has great significance for catalytic cracking, secondary and tertiary oil recovery and heterogeneous catalysis. We are using molecular simulation techniques in two distinct ways in this area of research.

One approach uses simple models to help us understand the influence of various factors, including the pore geometry and molecular structure on the system behavior. Real fluids have frequently been mod-

eled as a system of hard particles. Although simple, these potentials accurately represent the structure of real fluids. Moreover, they facilitate a direct comparison of the simulation results with purely theoretical approaches such as the Enskog kinetic theory. We are using molecular dynamics simulation to investigate the properties of a hard ellipsoid fluid, which serves as a model for *molecular* fluids, confined in various model micro-pores: a slit pore in which the fluid is trapped between two rigid planar walls at fixed separation, and isotropic pore structures modeled by configurations of overlapping spheres. The translational and rotational diffusion coefficients are evaluated for a range of molecular elongations, slit widths or porosities and densities. One interesting result of our preliminary studies is that the porous structure is selectively permeable to linear molecules relative to spheres. Moreover, the translational diffusion coefficient initially *increases* with increasing particle length before decreasing to zero at the percolation threshold.

In a second, more applied, area we are investigating the use of a chemically modified microporous silica medium for the separation of organic mixtures, such as methane and ethane In the new approach, the isolation of the components is based on their modified interactions with the silica surface instead of the molecular size differential. Experimental studies indicate that the adsorption isotherms of pure substances can be significantly influenced by chemical doping of the absorbate. In our work the microporous silica is modeled as a collection of microspheres and the selectivity of the medium is enhanced by randomly assigning a stronger interaction potential to a given fraction of the microspheres. We use molecular dynamics simulation to generate the trajectories of the gas molecules within the microporous medium from which the diffusivities and permeabilities are computed. In an initial study we have examined the transport characteristics of a equimolar mixture of methane and ethane for a range of temperatures. These results indicate that the selectivity of the medium may be enhanced without reducing its permeability. By manipulating the extent and type of doping, loading and temperature conditions we can optimize the separation. Once the optimum conditions are established, the membrane can be synthesized. However, the use of molecular simulation with realistic potential models can reduce the total cost by orders of magnitude compared with a purely experimental approach.

Molecular Simulation of Fluid Phase Equilibria: A quantitative description of the phase behavior of mixtures is often a prerequisite in the design of separation processes. In recent years, a number of significant developments in molecular simulation techniques suggest that the direct calculation of phase diagrams from molecular potential models is now a realistic proposition. For example, the Gibbs-Duhem integration technique for pure components involves integrating the Clapeyron equation along the coexistence line . The ordinary differential equation is solved with a predictor-corrector technique with the novel feature that the right hand side (containing the differences in enthalpy and volume of the two coexisting phases), is calculated by molecular simulation. A notable feature of the method is that it avoids the need for direct particle insertion, which can be problematic at high densities.

To extend the method to mixtures, one needs an analog of the Clapeyron equation, which can be developed within the formalism of the semi-grand ensemble. To integrate the Clapeyron-like equation we

use orthogonal collocation, which reduces the ODE to a set of coupled algebraic equations. From a computational perspective, the great advantage of this approach is that simulations of the coexisting phases at different compositions can be run in *parallel*, with significant reduction in the computational time compared with stepwise integration. In collaboration with Professor K. C. Chao and Peter Bereolos, we have successfully applied the method to Lennard-Jones binary mixtures, including some with azeotropes, and we are now applying the method to realistic potential models for methane/ethane and carbon dioxide/ethane mixtures .The new method is considerably faster than earlier computational approaches to phase equilibria and we expect that we will be able to examine the phase equilibria of industrially significant mixtures. Some useful potential models are already available for more complex molecules, but these have not yet been fully exploited as a result of the relative inefficiency of the previous approaches.

Publications

Ricci, S.M., J. Talbot and P. Viot, "Computation of the Free Area in Configurations of Anisotropic Particles," *Molecular Simulation,* 13**,** 1, (1994).

Ricci, S.M., J. Talbot, B. Senger, P. Schaaf and J.-C Voegel, "A Lattice Model for Protein Adsorption Kinetics," *J. Phys. Chem.,* 98**,** 4906-4912 (1994).

Viot, P., G. Tarjus, H.S. Choi and J. Talbot, "Restructuring Effects in the Irreversible Deposition of Spheres on a Plane," *Phys. Rev. E.,* 49**,** 3239 (1994).

Senger, B., P. Schaaf, J. Bafaluy, J. Talbot and J.-C. Voegel, "Adhesion of Hard Spheres Under the Influence of Double-Layer, van der Waals and Gravitational Potentials at a Solid/Liquid Interface," *Proc. Natl. Acad. Sci.,* 91, 3004-3008 (1994).

Jin, X., G. Tarjus and J. Talbot, "An Adsorption-Desorption Process on a Line: Kinetics of the Approach to Closest Packing," *J. Phys. A: Math. Gen.,* 27, L195-L200 (1994).

Talbot, J., X. Jin and N.-H. L. Wang, "New Equations for Multicomponent Adsorption Kinetics," *Langmuir,* 10, 1663-1666, 1994.

Boyer, D., J. Talbot, G. Tarjus, P. Van Tassel and P. Viot, "Exactly Solvable Models of Irreversible Adsorption with Particle Spreading,"*Phys. Rev. E.,* 49, 5525-5534 (1994).

Jin, X., J. Talbot and N.-H.L. Wang, "Analysis of Steric Hindrance Effects on Adsorption Kinetics and Equilibria," *AIChE Journal,* 40, 1685-1696 (1994).

Van Tassel, P., P. Viot, G. Tarjus and J. Talbot, "Irreversible Adsorption of Macromolecules at a Liquid-Solid Interface: The Effects of Conformational Change," *J. Chem. Phys.,* 101, 7064 (1994).

Ricci, S.M., J. Talbot, G. Tarjus and P. Viot, "A Structural Comparison of Random Sequential Adsorption and Equilibrium Configurations of Spherocylinders," *J. Chem. Phys.,* 101, 9164 (1994).

Choi, H.S., J. Talbot, G. Tarjus and P. Viot, "Percolation and Structural Properties of Particle Deposits," *Phys. Rev. E.,* 51(2) (1995).

Stamatopolou, A., L.E.S. de Souza, D. Ben-Amotz and J. Talbot, "Chemical Potentials of Hard Molecular Solutes in Hard Sphere Fluids. Monte Carlo Simulations and Analytical Approximations," *J. Chem. Phys., 102,* 2109 (1995).

Bafaluy, F.J., H.S. Choi, B. Senger and J. Talbot, "Effect of Transport Mechanisms on the Irreversible Adsorption of Large Molecules," *Phys. Rev. E., 51,* 5985 (1995).

Boyer, D., P. Viot, G. Tarjus and J. Talbot, "Percus-Yevick-like integral equation for Random Sequential Addition," *J. Chem. Phys.* (in press).

Talbot, J., "Time-Dependent Desorption: A Memory Function Approach," *Adsorption* (in press).

Bereolos, P., K.C. Chao and J. Talbot, "Simulation of Free Energy in the NPT Ensemble without Particle Insertion," *Mol. Phys.* (submitted).

Raghavan, K. and J. Talbot, "Gas Separation Using Chemically Modified Porous Membranes," *AIChE J* (submitted).

Van Tassel, J. Talbot, G. Tarjus and P. Viot, "The kinetics of irreversible adsorption with particle conformational change: A density expansion approach," *Phys. Rev. E.* (submitted).

Meeting Presentations

"Kinetics of Reversible Adsorption, AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Gas Separation Using Chemically Modified Porous Media," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Dynamics of a Hard Ellipsoidal Fluid in Porous Media," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"The Effects of Conformational Changes on the Adsorption of Biomolecules at the Liquid-Solid Interfaces," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Percolation and Structural Properties of Particle Deposits," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Percolation and Structural Properties of Particle Deposits," AIChE Annual Meeting, San Francisco, CA, November, 1994.

Invited Lectures

"Towards a Quantitative Understanding of Protein Adsorption Kinetics," Biozentrum, University of Basel, Basel, Switzerland, June, 1995.

Modelling the Adsorption of Proteins and Colloidal Particles," Department of Physics, Universitat Autònoma de Barcelona, June, 1995.

"Transport Properties of Fluids in Porous Media," Laboratoire de Physique Théorique des Liquides, Université Pierre et Marie Curie, Paris, France, June, 1995.

"Kinetics and Structure of Random Reversible Adsorption," Workshop on Space-Filling Problems, Ecole de Physique des Houches, Les Houches, France, January 9-19, 1995.

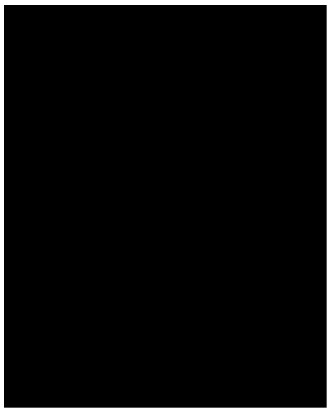
"Kinetics of Irreversible Adsorption with Applications to Proteins," Department of Chemical Engineering, University of Massachusetts, December 1, 1994.

"Kinetics of Reversible Adsorption," Department of Chemical Engineering, University of Massachusetts, December 1, 1994.

George T. Tsao

1974

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



Degrees

B.S., National Taiwan University, 1953

M.S., University of Florida, 1956

Ph.D., University of Michigan, 1960

Interests

Biochemical engineering

Renewable resource utilization

Publications

Le, Jean, L.B. Tsai, C.S. Gong, and G.T. Tsao, "Effect of Nitrogen Source on Xylitol Production by Candida sp.L-102," *Biotechnology Letters 17*, 167-170 (1995).

Lee, C.Y., J. Wen, S.N. Thomas, W.N. Delgass, J.B. Grutzner, and G.T. Tsao, "Conversion of Biomass to Ethanol: Isomerization of Xylose over HY Zeolite," *Applied Biochem. Biotechnol.* (in press).

Xia, Y., X. Yu, and G.T. Tsao, "Identification of Required Nutrient Components of Yeast Nitrogen Base for *Candida shehatae* Fermenting Xylose to Ethanol, "*Biotechnology Letters, 17,* 161-166 (1995).

Krishnan, M.S., G.T. Tsao, N. Kasthurikrishnan, N. Srinivasan, and R.G. Cooks, "Process Engineering of High Ethanol Tolerance Yeast for the Manufacture of Ethanol," *Applied Biochem. Biotechnol.* (in press).

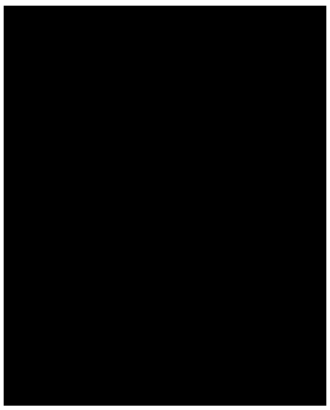
Lu, Z., C.W. Yang, and G.T. Tsao, "Fermentation of Xylose to Glycerol by *Rhizopus javanicus*," *Applied Biochem. Biotechnol*. (in press).

Yang, C.W., Z. Lu and G.T. Tsao, "Lactic Acid Production by Pellet-Form *Rhizopus oryzae* in A. Submerged System," *Applied Biochem. Biotechnol.* (in press).

Venkat Venkatasubramanian

1988

Associate Professor



Degrees

BTech., University of Madras, India, 1977

MS, Physics, Vanderbilt University, 1979

MS, Cornell, University, 1982

PhD, Cornell University, 1984

Interests

Intelligent Systems for Process Diagnosis and Supervisory Control

Process Hazards Analysis

Composite Products and Molecular Design

Knowledge-Based Systems, Neural Networks and Genetic Algorithms

Research Areas

A Framework for Integrating Process Monitoring, Diagnosis, and Control Tasks: Every day in process plants, process operators deal with the tasks of monitoring the process and assessing its current state, detecting and diagnosing any abnormal behavior, and taking the appropriate control actions. While these tasks are intimately related to each other and cannot really be treated as isolated tasks, typical approaches in the past have looked at monitoring, diagnosis, and control problems separately. In this project, we have developed a conceptual framework for addressing these issues in an integrated manner. This project addresses two kinds of integration that are needed for a satisfying solution to this process management problem: (i) the integration of tasks, namely, monitoring, diagnosis, and control and (ii) the integration of solution approaches. The solution approaches we focus upon in this project are knowledge-based systems and neural networks.

A Knowledge-Based Approach for Automating Hazard and Operability Analysis: Hazard and operability (HAZOP) analysis is the study of systematically identifying every conceivable deviation, all the possible abnormal causes for such deviation, and the adverse hazardous consequences of that deviation in a chemical plant. Such an analysis is often carried out by a group of experts poring over the process P&IDs for weeks, applying a set of "guide words" to the process variables associated with each process line and equipment and finding the causes and consequences for those process variable deviations. Thus, Hazop analysis is a very difficult, labor-intensive, and time-consuming process. An automated hazop system can cut down on the time and effort involved in performing a hazop review, make the review more thorough, complete, and detailed, and minimize or eliminate human errors.

In this project, we have developed a knowledge-based framework by recognizing and exploiting two important features of the HAZOP analysis: (i) even though each HAZOP analysis is unique to a process, it is systematic and logical; and (ii) many aspects of the analysis are the same for different process flow sheets. Thus, HAZOP analysis can be automated through the use of knowledge-based systems. We have developed a knowledge-based system, called *HAZOPExpert*, that separates the knowledge base into "process specific" and "process general" knowledge. Process specific knowledge consists of the properties of process materials, type of the particular reactions carried out, materials of construction of the equipments, etc. Process general knowledge consists of unit models for different process equipment and would model behavioral knowledge about causes, consequences and propagation of process deviations. An object-oriented framework is being used for this framework. Currently research is in progress to develop this framework further to include complex process units and flowsheet configurations as seen in real-life industrial settings.

Designing Engineering Polymers: The traditional process of designing new molecules that possess certain desired properties often requires a search involving an enormous number of potential candidate molecules. It is an elaborate and expensive iterative process with the chemist or chemical engineer hypothesizing a compound, synthesizing the material, testing for desired properties, and redesigning if the desired properties are not met. In this project, we have developed a framework for the modeling and automation of this product design process using a combination of neural networks and genetic algorithmic techniques. The two primary components of this approach are: (i) a property prediction component for evaluating candidate molecules and (ii) a component for identifying potential candidate polymers. Current procedures for property prediction, such as group contribution methods, assume the physicochemical properties depend in a straightforward manner on chemical structure. These methods, however, are generally unable to capture the complex interactions between various descriptors of molecular architectures which give rise to a specific engineering property. Neural networks offer a more suitable approach for describing such complex nonlinear structure-property relationships and are used for the forward mapping problem. The search for novel polymer candidates is carried out by using genetic algorithms. By a judicious combination of mutation and crossover operators, and the appropriate polymer chemistry constraints, an effective search can be carried out.

Publications

Venkatasubramanian, V., K. Chan and J. M. Caruthers, "Evolutionary Large Scale Molecular Design Using Genetic Algorithms," *J. Chem. Info. and Comp. Sci.*, 35, 188-195 (1995).

Rengaswamy, R. and V. Venkatasubramanian, "A Syntactic Pattern Recognition Approach for Process Monitoring and Fault Diagnosis," *Engineering Applications of Artificial Intelligence Journal*, 8(1), 35-51 (1995).

Venkatasubramanian, V., K. Chan and J. M. Caruthers, "A Genetic Algorithm Approach for Computer-Aided Molecular Design," in *ACS Symposium Series Volume on Applications of Computer-Aided Molecular Design*, C. Reynolds, K. Holloway, and H. Cox (Eds.), The American Chemical Society (1995).

Venkatasubramanian, V. and R. Rengaswamy, "Clustering and Statistical Techniques in Neural Networks," in *Neural Networks in Chemical Engineering*, A. Bulsari (Ed.), Elsevier (1995).

Aoyama, A., F. J. Doyle, and V. Venkatasubramanian, "Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control," *J. of Process Control* (in press) 1995.

Aoyama, A., F. J. Doyle, and V. Venkatasubramanian, "Control-Affine Neural Network Approach for Nonminimum-Phase Nonlinear Process Control," *J. of Process Control* (in press) 1995.

Aoyama, A., F. J. Doyle, and V. Venkatasubramanian, "Fuzzy Neural Networksfor Nonlinear Process Control," E*ngg. Applns. of Art. Intel.* (in press) 1995.

Vaidhyanathan, R. and V. Venkatasubramanian, "Digraph-based Models for Automated HAZOP Analysis," *J. of Rel. Engg. and Sys. Safety* (in press) 1995.

Invited Lectures

"Towards Integrated Process Supervision: Current Trends and Future Directions," in the Proceedings of the *Second IFAC International Conference on AI/KBS in Process Control,* University of Lund, Lund, Sweden, August, 1994. (Keynote Address)

"AI Approaches to Computer-aided Molecular Design," The American Physical Society Annual Meeting, San Diego, CA, March, 1995.

"Neural Networks and Genetic Algorithms for Molecular Design," *International Conference on Genetic Algorithms and Neuralworks for Drug Design*, Lyon, France, June 10-12, 1995.

Automating HAZOP Analysis, Dept. of Automatic Control, Technical University of Lund, Lund, Sweden, August, 1994.

AI Applications in Process Safety and Product Design, Eli Lilly and Co, Indianapolis, IN, September, 1994.

Computer-Aided Molecular Design Using Neural Networks and Genetic Algorithms, Dow Elanco, Indianapolis, IN, October, 1994.

A Hybrid Framework for Real-time Process Fault Diagnosis, Honeywell Technical Center, Minneapolis, MN, March, 1995.

AI Methods for Materials Formulation and Design, The Lubrizol Corporation, Cleveland, OH, April, 1995.

Chaired Conferences/ Symposia

Intelligent Manufacturing Systems session, AIChE Annual Meeting, St. Louis, MO, November, 1994 (co-chairman).

Member of the International Advisory Board, Ninth International Conference on *Artificial Intelligence Applications in Engineering,* Toulouse, France, July, 1994.

International Conference on *Intelligent Systems in Process Engineering (ISPE'95)*, Snowmass, CO, July 9-14, 1995 (co-chairman).

Meeting Presentations

"Evolutionary Molecular Design," in the Proceedings of the *International Conference on Foundations of Computer Aided Process Design, FOCAPOD93*, Snowmass, CO, July, 1994.

"Automated Development of Causal Models for Fault Diagnosis," AIChE Annual Meeting, San Francisco, CA, November, 1994.

"Interactive Molecular Design," AIChE Annual Meeting, San Francisco, CA, November, 1994.

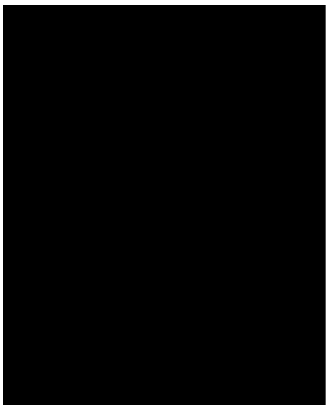
"AI Approaches to Computer-aided Molecular Design," The American Physical Society Annual Meeting, San Diego, CA, March, 1995.

"A Hybrid Apparoach to Process Fault Diagnosis," AIChE Annual Meeting, Atlanta, GA, March, 1995.

Nien-Hwa Linda Wang

1980

Professor



Degrees

BS National Taiwan University, 1971.

MS University of Wyoming, 1973.

PhD University of Minnesota, 1978.

Interests

Biochemical Separation and Purification

Biochemical Adsorption

Multicomponent ion exchange/adsorption and Large Scale Chromatography

Environmental Applications of Separation Techniques

Mass transfer in biological systems

Awards and Major Appointments

NSF Faculty Award for Women Scientists and Engineers (1991-1996).

Member of NIH Study Section of Surgery and Bioengineering.

Research Areas

Simulations of Chromatography Processes for Biochemicals: Mixtures of large biochemicals can exhibit complex chromatographic behavior. In addition to mass transfer mechanisms, the presence of nonequilibrium adsorption/desorption, aggregation, denaturation and other solution or solid phase reactions can be important. A VErsatile Reaction-SEparation model for Liquid Chromatography applications (VERSE-LC) which considers all these nonequilibrium effects has been developed. The VERSE-LC model equations are spatially discretized by orthogonal collocation on finite elements and the resulting ordinary differential equations are solved in time by a differential/algebraic system solver. Convergence criteria are established for each type of nonequilibrium simulation. A general dimensionless group approach is presented to determine the controlling rate process and thus predict the character of the effluent history. The VERSE-LC model can treat systems with various adsorption mechanisms, and can simulate frontal, isocratic and gradient elution, displacement chromatography, as well as combinations of these modes. VERSE-LC is useful for gaining a fundamental understanding of complex protein chromatography, for scaling with respect to flow rate, particle size and feed concentration, and for exploring new designs of large scale chromatography. Several US companies and academic laboratories have licensed VERSE-LC from Purdue.

Publications

Whitley, R., X. Zhang, and N.-H.L. Wang, "Protein Denaturation in Nonlinear Isocratic and Gradient Elution Chromatography," *AIChE J. 40* (6), 1067-1084 (1994).

Talbot, J., X. Jin, and N.-H.L. Wang, "New Equations for Multicomponent Adsorption Kinetics," *Langmuir, 10,* 1663-1666 (1994).

Jin, X., J. Talbot, and N.-H.L. Wang, "Analysis of Steric Hindrance Effects on Adsorption Kinetics and Equilibria," *AIChE J.*, 40 (10), 1685-1696 (1994).

Hoffman, C.M., E.N. Houstis, J.R. Rice, A.C. Catlin, M. Gaitatzes, S. Weerawarana, N.-H.L. Wang, C.G. Takoudis, and D.G. Taylor, "Softlab - A Virtual Laboratory for Computational Science," *Mathematics and Computers in Simulation*, 36, 479-491 (1994).

Clark, W.R., W. L. Macias, B.A. Molitoris, and N.-H.L. Wang, "Membrane Adsorption of Beta 2-Microglobulin: Equilibrium and Kinetic Characterization," *Kidney International*, 46, 1140-1146 (1994).

Clark, W.R., W. L. Macias, B.A. Molitoris, and N.-H.L. Wang, "Plasma Protein Adsorption to Highly Permeable Hemodialysis Membranes," (in press) 1995.

*Koh, J.-H., N.-H.L. Wang, and P.C. Wankat, "Amino Acid Recovery Using Fluidized Ion Exchange Bed," *IEC Research* (in press) 1995.

Franses, E.I., F.A Siddiqui, D.J. Ahn, C.-H. Chang, and N.-H.L. Wang, "Thermodynamically Consistent Equilibrium Adsorption Isotherms for Mixtures of Different-Size Molecules," *Langmuir* (accepted).

Chaired Conferences/ Symposia

Chairman of the Symposium on Advances in Bioseparations, AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994.

Meeting Presentations

"Orientation Effects of Adsorbed Molecules on Isotherms and Column Adsorption Dynamics," Z. Ma, X. Jin, and N.-H.L. Wang, Symposium on Fundamentals of Adsorption and Ion Exchange, 1994 AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994.

"Comparison of Surface and Pore Diffusion in Multicomponent Large Scale Chromatography," Z. Ma (speaker), R. Whitley, and N.-H.L. Wang, Symposium on Recent Developments in Adsorption and Ion Exchange, 1994 AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994.

"Kinetics of Reversible Adsorption Processes," J. Talbot (speaker), X. Jin, and N.-H.L. Wang, Symposium on Molecular Theory of Adsorption Equilibria and Kinetics, 1994 AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994.

"Isolation and Purification of Taxol from Plant Tissue Culture Media Using Preparative Chromatography," B. Au (speaker), Z. Ma, and N.-H.L. Wang, Symposium on Strategies for Recovery Biological Molecules, 1994 AIChE Annual Meeting, San Francisco, CA, Nov. 13-18, 1994.

"VERSE-LC: Modeling of Large Scale Chromatography and Adsorptive Separations," R.D. Whitley (presenter of poster), Z. Ma, M.V. Ernest, D.J. Wu, and N.-H.L. Wang, 13th International Symposium on Preparative Chromatography, Washington, DC, June 11-14, 1995.

Invited Lectures

"Environmental Applications of Ion Exchange and Adsorption," Environmental Engineering, Purdue University, West Lafayette, IN, October, 14, 1994.

"Environmental Applications of Ion Exchange and Adsorption," Westinghouse Savannah River Co., Aiken, SC, April, 19, 1995.

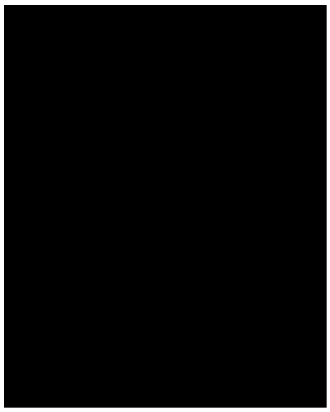
"Competitive Chemical and Biochemical Ion Exchange and Adsorption in Chromatography Systems," Alcon Laboratories, Fort Worth, TX, May 25, 1995.

"Comparison of Pore and Surface Diffusion in Multicomponent Adsorption and Liquid Chromatography Systems," 13th International Symposium on Preparative Chromatography, Washington, DC, June 11-14, 1995.

Phillip C. Wankat

1970

Professor and Head of Freshman Engineering



Degrees

BS, Purdue University, 1966

PhD, Princeton University, 1970

MSEd, Purdue University, 1982

Interests

Adsorption and Chromatography

Simultaneous fermentation/separation

Distillation

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 and thermal swing regeneration methods are being explored.

Other separations research in progress: Staged fluidized bed ion exchange chromatography systems for purification of biochemicals which can handle feeds with particulates such as cell fragments are being developed. Studies of simultaneous fermentation/separation have shown that the reaction can be driven to completion with higher overall reaction rates. Methods to improve distillation and make it more energy efficient are being explored.

Publications

Koh, J.-H., N.-H.L. Wang, and P.C. Wankat, "Ion-Exchange of Phenylalanine in Fluidized/Expanded Beds," *Ind. Engr. Chem. Research* (in press).

Simms, C, Arumugam, B., and P.C. Wankat, "Modified Displacement Chromatography Cycles for Gas Systems," *Chem. Engr. Sci.* (in press).

Venkatesh, K.V., P.C. Wankat, and M.R. Okos, "Kinetic Model for Lactic Acid Production From Cellulose by Simultaneous Fermentation and Sacharification," *AIChE Symp. Ser., 300*, 80-87 (1994).

Hatton, D.M., W.K. LeBold, and P.C. Wankat, "Proactive Counseling Measures with Freshman Engineering Students," *Proceedings ASEE Annual Conference*, ASEE, Washington, DC (in press) 1995.

Editorial Boards

Separation and Purification Methods, Editor-in-Chief.

Adsorption.

Chemical Engineering Education.

Separation Science and Technology.

Invited Lectures

"Improving Lectures," Civil Engineering, Purdue University, September 2, 1994; University of Toledo, Toledo, OH, May 24, 1995; University of Colorado-Boulder, April 20, 1995.

"Improving Lectures," Young Faculty Forum, AIChE Meeting, San Francisco, CA, November, 1994.

"The Cloudy Crystal Ball: The Future of Engineering Education," North Carolina State University, Raleigh, NC, March 27, 1995.

"The Efficient Professor," live TV broadcast by NTU to 75 sites, May 9, 1995.

Projects Funded

Award Amount	PI/Sponsor/Title	Project Period
$160,000	**L.F. Albright** National Science Foundation Alkylation of Isobutane with Light Olefins: Clarification of Chemistry and Physical Phenomena	09/93-08/96
$291,608	**R.P. Andres** Army Research Office Electronic Conduction in Molecular Nanostructures	07/92-06/96
$366,426	**R.P. Andres** **J. Talbot** **R. Reifenberger** National Science Foundation Synthesis of Nanometer Diameter Particles and Measurement of Particle-Particle and Particle Substrate Interactions	05/92-05/96
$65,396	**R.P. Andres** Arco Chemical Co. Development of Selective Catalyst for Proplyene Epoxidation	05/95-05/97
$22,000	**R.P. Andres** **W.N. Delgass** Trask Trust Fund Support for Exploratory Research	09/94-09/95
$10,000	**O.A. Basaran** Exxon Education Foundation Research into Micron-and Sub-Micron Size Particles	10/94-09/95
$284,995	**J.M. Caruthers** **K.C. Chao** **V. Venkatasubramanian** DIPPR/AICHE Handbook of Diffusion and Thermal Properties for Polymer Solutions	01/92-12/94
$20,350	**J.M. Caruthers** Purdue Research Foundation A Solid State NMR Study of Molecular Mobility in Polymeric Glasses	05/93-04/95
$157,885	**J.M. Caruthers** **H.S. Lackritz** **N.A. Peppas** National Science Foundation Undergraduate Materials Education Initiative: An Innovative U/G Materials Curriculum	10/92-09/95

Award Amount	PI/Sponsor/Title	Project Period
$173,214	**J.M. Caruthers** National Science Foundation Engineering Research Center & CIDMAC Intelligent Manufacturing for Advanced Composites	02/93-09/95
$62,718	**J.M. Caruthers** AFOSR Fundamental Models for Predicting Lifetime Performance of High Performance Polymeric Materials	03/95-03/96
$10,200	**J.M. Caruthers** Purdue Research Foundation Phase Equilibria of Polymer Mixtures	03/95-96
$11,992	**J.M. Caruthers** Class of 1941 Teaching Innovation Grant Development of Computer Simulation Modules for Teaching	05/95-99/99
$24,800	**K.C. Chao** Purdue Research Foundation Thermodynamic Properties of Polymer Melts and Solutions	03/93-02/95
$15,000	**W.N. Delgass** Exxon Education Foundation Catalysis on Transient Kinetics of Ethylene Epoxidation	08/92-03/95
$199,909	**W.N. Delgass** **G.T. Tsao** U.S. Department of Energy Zeolite Catalyses in Conversion of Cellulosies	02/92-02/95
$20,400	**W.N. Delgass** Purdue Research Foundation Solid State NMR Characterization of Vanadium Zeolite Catalysis for No Reduction	04/94-03/96
$97,902	**W.N. Delgass** National Science Foundation Engineering Research Center and CIDMAC Temperature Sensors for Intelligent Manufacturing Systems	02/93-09/95
$25,000	**W.N. Delgass** Dupont Central Research & Development Research for Expanding the Horizons and Overall Understanding of Heterogeneous Invited Lectures Catalysis	12/94-99/99

Award Amount	PI/Sponsor/Title	Project Period
$10,000	**W.N. Delgass** Exxon Education Foundation Solid Acid Catalysis in Liquid Media	02/95-99/99
$212,500	**F.J. Doyle** National Science Foundation NSF/NYI Matching Funds	03/94-99/99
$25,252	**F.J. Doyle** National Science Foundation Tools for the Deployment of Computer Integrated Process Operations Research to Chemical Engineering Curriculum and Industrial Practice	09/93-02/95
$224,425	**F.J. Doyle** National Science Foundation Nonlinear Dynamic Analysis of a Biological Control Mechanism for Applications in Process Modeling and Control	09/93-09/96
$50,000	**F.J. Doyle** **N.A. Peppas** Showalter Trust Insulin Response & Delivery Using CDD Device for the Treatment of Diabetes Mellitus	06/94-09/95
$10,200	**F.J. Doyle** Purdue Research Foundation Specialized Mathematical Programming Methods in the Model Predictive Control of Large Scale Systems	04/95-96
$7,983	**E.I. Franses** Elsevier Science Publishers B.V. Colloids and Surfaces A: Physicochemical and Engineering Aspects	12/92-99/99
$240,000	**E.I. Franses** National Science Foundation Adsorption Dynamics of Mixed Surfactants and Proteins at Air/Water Interfaces: Applications to Foams and Lung Surfactant	08/93-07/96
$20,400	**E.I. Franses** Purdue Research Foundation Engineering Design of Lung Surfactant Formulations	05/94-04/96

Award Amount	PI/Sponsor/Title	Project Period
$116,300	**E.I. Franses** **H.S. Lackritz** National Science Foundation Engineering Research Equipment Grant Dynamic Spectroellipsometer for Reaction and Adsorption Measurements	09/93-08/95
$ 56,287	**R.A. Greenkorn** Indiana Dept. of Environmental Management Indiana Pollution Prevention Institute	06/94-06/95
$42,874	**R.A. Greenkorn** Showalter Trust The Movement of Pollutants Underground	06/94-06/96
$311,657	**H.S. Lackritz** Air Force Office of Scientific Research Nonlinear Optical and Charge Distribution Studies Probing Electric Field Effects in Polymer Thin Films for Second Order Nonlinear Optics	05/93-04/96
$15,000	**H.S. Lackritz** Exxon Education Foundation Minority Student Tutoring	08/92-07/95
$170,000	**H.S. Lackritz** National Science Foundation Charge Distribution & Nonlinear Optical Studies Probing Electric Field Effects in Polymer Thin Films	01/93-01/96
$200,000	**H.S. Lackritz** National Science Foundation NSF Presidential Faculty Fellows Program	08/93-07/95
$375,000	**H.S. Lackritz** Office of Naval Research High Temperatures Polymers for Second Order Nonlinear Optics: Photorefractive Polyimides for Photonic Materials	04/92-04/97
$90,000	**H.S. Lackritz** Office of Naval Research High Temperature Polymers for Second Order Nonlinear Optics: Photo Refractive Polymide for Photonic Materials	06/93-96
$93,659	**H.S. Lackritz** AFOSR Characterization of Optical Properties of Thin Nonlinear Optical Polymer Films for Device Applications as a Function of Processing	06/95-98

Award Amount	PI/Sponsor/Title	Project Period
$25,000	**H.S. Lackritz** Lockheed Missles/AFOSR Electro-Optic Polymer Development Contract	02/95-01/96
$312,500	**J.F. Pekny** National Science Foundation/Industry Presidential Young Investigator Award	08/90-09/95
$23,800	**J.F. Pekny** Purdue Research Foundation Combinatorial Optimization for Molecular Simulation and Design	03/93-02/95
$240,501	**J.F. Pekny** **G.V. Reklaitis** NSF A Comprehensive Approach to Chemical Process Scheduling Problems	04/94-08/97
$13,960	**J.F. Pekny** Advanced Process Combinatorics Towards a Practical Distributed System for Solving Mixed Integer Linear Programming Problems: Resolving Algorithmic Issues in Performance Enhancement and a Minimal Interfaces for Providing	10/94-03/95
$5,000	**N.A. Peppas** International Association for Pharmaceutical Tech. European Journal of Pharmaceutics and Biopharmaceutics	10/93-99/99
$214,218	**N.A. Peppas** National Science Foundation Polymer Dissolution	09/92-09/95
$189,820	**N.A. Peppas** National Science Foundation Multifunctional Polymerization Kinetics and Network Structure Thereof	08/93-08/96
$9,496	**N.A. Peppas** National Science Foundation Multifunctional Polymerization Kinetics and Network Structure Thereof	08/93-08/96
$6,025	**N.A. Peppas** NATO (N. Atlantic Treaty Organization) Investigation of Water and Solute Diffusion in Hydrophilic Polymers	03/94-02/96

Award Amount	PI/Sponsor/Title	Project Period
$556,596	**N.A. Peppas** PHS-NIH National Institute of General Medical Science Mucoadhesive Polymers for Nasal and Buccal Drug Delivery	05/91-09/95
$24,350	**N.A. Peppas** Purdue Research Foundation Kinetics of Multimethacrylate Polymerizations and Structural Analysis of Network Thereof	03/93-02/95
$60,000	**N.A. Peppas** Showalter Trust Showalter Distinguished Professorship in Biomedical Engineering	11/93-06/95
$194,876	**D. Ramkrishna** U.S. Dept. of Agriculture Investigation of Shelf-Life of Food Emulsions	09/92-09/95
$45,000	**D. Ramkrishna** American Institute of Chemical Engineers Investigation of Shelf-Life of Food Emulsions	05/92-04/96
$20,400	**D. Ramkrishna** Purdue Research Foundation Biodegradation of Aromatic Hydrocarbons	05/94-04/96
$90,954	**D. Ramkrishna** Office of Naval Research Modelling of Microbiological Remediation of Shipboard Waste Effluents	04/94-95
$204,924	**G.V. Reklaitis** Shell Companies Foundation, Inc. Shell Oil Company Foundation Fellowship	09/85-08/95
$21,000	**G.V. Reklaitis** Camille & Henry Dreyfus Foundation, Inc. Multi-Media Instructional Aids for an Advanced Laboratory Course	01/94-12/95
$151,600	**G.V. Reklaitis** E.I. DuPont de Nemours & Company E.I. DuPont de Nemours & Company Fellowhsip	09/81-08/95
$1,688,892	**G.V. Reklaitis** U.S. Department of Education Purdue Program for Graduate Assistance in Chemical Engineering Areas of National Need	09/92-08/95

Award Amount	PI/Sponsor/Title	Project Period
$71,189	**G.V. Reklaitis** C.D. McAllister Endowment Goddard Fellowship	06/90-99/99
$337,500	**G.V. Reklaitis** National Science Foundation Renovation of Advanced Materials Laboratory in Chemical Engineering	03/94-05/95
$90,750	**G.V. Reklaitis** National Consortium Graduate Minorities Engineering & Science National Consortium for Minorities Fellowship	09/92-08/95
$59,572	**G.V. Reklaitis** Oak Ridge Associated Universities Computational Science Graduate Fellowship Program	09/92-08/95
$200,000	**G.V. Reklaitis** Phillips Petroleum Eastman Chemical Company Eli Lilly & Company Morton International Weyerhaeuser Company Computer Aided Process Operations Center (CIPAC)	05/93-99/99
$150,000	**G.V. Reklaitis** **R.G. Squires** Procter & Gamble Company Procter & Gamble Chemical Engineering Education Module	07/93-06/96
$69,716	**G.V. Reklaitis** Eli Lilly & Company Antibiotic Recovery from Fermentation Broth	08/94-03/95
$88,600	**E.M. Sevick-Muraca** National Science Foundation National Young Investigator Biomedical Optical Imaging	09/94-09/96
$168,773	**E.M. Sevick-Muraca** Public Health Service N.H. Frequency-Domain Photon Migration Imaging for Breat Cancer Screening	08/94-05/96
$10,600	**E.M. Sevick-Muraca** Vanderbilt University Optical Imaging in Tissues Using Measurement of Time-Dependent Photon Migration	08/94-04/95

Award Amount	PI/Sponsor/Title	Project Period
$49,576	**E.M. Sevick-Muraca** Mallinckrodt Medical Contrast Agents for Biomedical Optical Imaging	08/94-09/95
$22,728	**E.M. Sevick-Muraca** University of Tennessee Process Monitoring with Measurement of Photon Migration	09/94-08/95
$96,626	**R.G. Squires** Multi-sponsored Industry Study to Develop Chemical Engineering Laboratory Projects	10/87-99/99
$81,660	**R.G. Squires** National Science Foundation Educational Applications of Computer Simulations of Chemical Engineering Processes	02/94-02/96
$245,940	**C.G. Takoudis** **G.W. Neudeck** **E.P. Kvam** National Science Foundation REU Site for Microelectronic Materials and Processing	05/92-05/96
$415,000	**C.G. Takoudis** **M.J. Weaver** National Science Foundation Raman Spectroscopic Characterization of Transition-Metal Surfaces in Catalytic Reactor Systems	09/93-08/96
$125,000	**C.G. Takoudis** National Science Foundation Selective Epitaxial Growth of Silicon in a Chemical Vapor Deposition Reactor Part of a project: Softlab - A Laboratory for Computational Science, with Computer Science Department	10/92-09/97
$130,000	**C.G. Takoudis** **R. Uzsoy** National Science Foundation Integrating Process Fundamentals, Facility Design and Production Control of Semiconductor Manufacturing Systems	10/93-09/96

Award Amount	PI/Sponsor/Title	Project Period
$290,000	**C.G. Takoudis** **G.W. Neudeck** **E.P. Kvam** National Science Foundation Constrained Epitaxial Growth of Si-Based Heterostructures	09/93-08/96
$50,000	**J. Talbot** American Chemical Society Transport of Molecular Fluids in Porous Media	01/94-08/96
$20,250	**J. Talbot** Purdue Research Foundation Molecular Dynamics of Nanoclusters	09/93-04/95
$17,550	**J. Talbot** National Science Foundation Theoretical Studies of Irreversible Adsorption at the Solid Liquid Interface	04/95-98
$71,106	**G.T. Tsao** USDA Value Added Products from Steep Water and Residual Fiber Corn Wet Milling Process	09/92-09/94
$57,772	**G.T. Tsao** U.S. Department of Energy Zeolite Catalysis in Conversion of Cellulosies	09/92-09/94
$10,000	**V. Venkatsubramanian** Arthur D. Little, Inc. Hazopexpert Project	08/93-12/95
$309,149	**V. Venkatsubramanian** National Science Foundation Process Fault Diagnosis and Control Using Neural Networks	09/90/08-94
$370,210	**V. Venkatasubramanian** PHS-CDC National Institute of Occupation, Safety and Health A Knowledge-Based Framework to Automate Hazop Analysis	09/93-09/95
$10,200	**V. Venkatasubramanian** Purdue Research Foundation Computer-Aided Molecular Design Using Genetic Algorithms	11/94-99/99

Award Amount	PI/Sponsor/Title	Project Period
$144,000	**N.-H.L. Wang** **M.R. Okos** U.S. Department of Agriculture Food and Agricultural Sciences National Needs Graduate Fellowship Program	09/89-08/94
$173,570	**N.-H.L. Wang** Westinghouse Savannah River Co. Design & Development of Ion Exchange Processes for Removal and Concentration of Metal Ions in Liquid Nuclear Waste	06/94-05/96
$96,287	**N.-H.L. Wang** National Science Foundation Equipment for Measurement of Dynamic Adsorption of Proteins and Lipids at Air/Water Interfaces - Applications to Foams in Bioprocessing	11/92-10/94
$300,000	**N.-H.L. Wang** National Science Foundation NSF Faculty Awards for Women Scientists and Engineers	11/91-10/95
$20,350	**N.-H.L. Wang** Purdue Research Foundation Development of a Recovery and Purification Process for Taxol from Plant Tissue Culture Media	05/93-04/95
$17,000	**N.-H.L. Wang** Trask Trust Fund Beta-Site Testing and Further Development of Verse	01/93-12/95
$43,981	**N.-H.L. Wang** National Science Foundation Nonlinear Chromatography Part of a project: Softlab - A Laboratory for Computational Science, with Computer Science Department	02/93-09/94
$120,485	**P.C. Wankat** National Science Foundation Multicomponent Adsorption Processes	05/94-04/96
$23,800	**P.C. Wankat** **N.-H.L. Wang** Purdue Research Foundation Fluidized Bed Ion Exchange of Proteins	03/93-02/95
$50,000	**J.M. Wiest** **N.A. Peppas**	07/94-07/95

Award Amount	PI/Sponsor/Title	Project Period
	E.I. Franses **W.N. Delgass** **H.S. Lackritz** **J.F. Pekny** **V. Venkatasubramanian** National Science Foundation An REU Site for New Directions in Chemical Engineering	

Thesis Projects

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Bell, Cristi Lynn *N.A. Peppas*	Water and Solute Transport in Responsive Hydrogels of Poly (ethylene glycol) and Poly (methacrylic acid)	PhD August 5, 1994
Brazel, Christopher S. *N.A. Peppas*	Synthesis and Characterization of pH- and Temperature-Sensitive Hydrogels for Controlled Release of Antithrombotic Agents	MS August 5, 1994
Dietz, James Eric *N.A. Peppas*	Physical and Mechanical Characterization of Multifunctional (Meth) Acrylates	PhD August 5, 1994
Hsu, Sheng Tsiung *G.T. Tsao*	Design and Dynamics of Large Scale Chromatographic Processes	PhD August 5, 1994
Jurman, Kathleen Ann *W.N. Delgass*	Investigation of Pt and Pt/Rh HCN Catalyst Recrystallization with Scanning Tunneling Microscopy	PhD August 5, 1994
Lee, Ching-Yi *G.T. Tsao*	Isomerization of Xylose over Zeolites	PhD August 5, 1994
Lee, I-Ming (Ryan) *C.G. Takoudis*	Thermodynamic and Kinetic Studies of Silicongermanium Chemical Vapor Desposition and Characterization of the Grown Films by Ellipsometry	MS August 5, 1994
Watson, Bradley S. *K.C. Chao and R.A. Greenkorn*	Phase Coexistence and Free Energy Calculations by Monte Carlo Simulations	PhD August 5, 1994
Yasuda, Ken Eric *D. Ramkrishna*	Manipulation of Selectivity of Reactions in Liquid-Liquid Systems by Control of Dispersion Processes	MS August 5, 1994
Aoyama, Atsushi *V. Venkatasubramanian*	Modeling and Control of Nonlinear Processes Using Neural Networks and Fuzzy Logic	PhD December 17, 1994
Beck, Scot Brian *J.M. Caruthers*	Temporal and Spatial Analysis of Glass Transition Phenomena Using a Molecular Dynamics Study of Lennard-Jones Chains	PhD December 17, 1994
Clark, William Richard *N.-H.L. Wang*	Plasma Protein Adsorption to Highly Permeable Hemodialysis Membranes	MS December 17, 1994
Crane, Robert Andrew *R.P. Andres*	Synthesis and Characterization of Selective Oxidation Catalysts	MS December 17, 1994
Ernest, Jr., Michael Vance *N.-H.L. Wang*	Development of Ion Exchange Processes for Decontamination of Cesium-137 from Alkaline Nuclear Waste	MS December 17, 1994

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Kendi, Thomas A. *F.J. Doyle, III*	Nonlinear Control Using Approximate Linearization Techniques	MS December 17, 1994
Krishnan, Mahesh Subramaniam *G.T. Tsao*	Process Engineering of High Ethanol Tolerance Yeast for the Manufacture of Ethanol	MS December 17, 1994
Kurdikar, Devdatt L. *N.A. Peppas*	Multifunctional Polymerization Kinetics and Network Structure Thereof	PhD December 17, 1994
Narang, Atul *D. Ramkrishna*	The Dynamics of Microbial Growth on Mixtures of Substrate	PhD December 17, 1994
Novenario, Carlos R. *K.C. Chao and R.A. Greenkorn*	Vapor-Liquid Equilibrium and Thermo-physical Property Predictions from the Chain-of-Rotators Equation of State	MS December 17, 1994
Osifchin, Richard G. *R.P. Andres*	The Production of Novel Electronic Structures Built with Coupled Nanometer-Diameter Metal Cluster Assemblies	PhD December 17, 1994
Paithankar, Dilip Yeshwant *R.P. Andres*	Atomistic Simulations of Nanometer Size Size Metal Clusters	PhD December 17, 1994
Pasmore, Tom A. *H.S. Lackritz*	Monte Carlo Simulation of Charge Transport Through Molecularly Doped Polymer Thin Films	MS December 17, 1994
Sathyagal, Arun N. *D. Ramkrishna*	Self-similarity in Drop Break-up Phenomena in Liquid-Liquid Dispersions Identification of Break-up Functions by Inverese Problem Approach	PhD December 17, 1994
Scott, Gregory Ball *W.N. Delgass*	An X-ray Photospectroscopic Modelling Technique for the Determination of Thin Medal Oxide Films	MS December 17, 1994
Au, Bob Wayne *N.-H.L. Wang*	Studies for the Design of a Recovery and Purification Process for Taxol from Plant Tissue Culture Broth	MS May 6, 1995
Chen, Ai-Qi *K.C. Chao*	Polymer Solution Phase Behavior Modeling by Chain-of-Rotators Equation of State	PhD May 6, 1995
Choi, Ho Suk *J. Talbot*	Irreversible Adsorption of Macromolecules at the Solid-Liquid Interface: Simulation and Theory	PhD May 6, 1995
Coltharp, Karen A. *E.I. Franses*	Dynamic Surface Tension Behavior of Aqueous Solutions and Dispersions of Sodium Soaps	MS May 6, 1995

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Colucci, Dina Marie *J.M. Caruthers*	The Effect of Temperature and Deformation on the Relaxation Behavior in the Glass Transition Region	PhD May 6, 1995
Curliss, David Brian *J.M. Caruthers*	^{15}N NMR Spectroscopic Investigation of Cure and Degradation of Imide Polymers	PhD May 6, 1995
Gooding, William B. *J.F. Pekny*	Specially Structure Formulations and Solution Methods for Optimization Problems Important to Process Scheduling	PhD May 6, 1995
Khan, Kamran *N.-H.L. Wang*	Biomolecule Adsorption in Immobilized Metal Ion Affinity Chromatography	MS May 6, 1995
McGinnis, Jerry K. *L.F. Albright and R.E. Eckert*	Investigation of Emulsions Involving Concentrated Sulfuric Acid and Hydrocarbons	MS May 6, 1995
Park, Sun Young *E.I. Franses*	Effects of Dispersion State and Surface Composition on the Dynamic Surface Tension Behavior of Sparingly Soluble Surfactant Systems	PhD May 6, 1995
Perkins, Matthew M. *R.A. Greenkorn*	An Examination of a Multiscale Volume Averaging Theory and a Stochastic-Nonlocal Theory for Modeling Dispersion in Scale-Dependent Porous Media	MS May 6, 1995
Pirog, Theodore W. *D. Ramkrishna*	Studies of Coalescence in Food Emulsions	MS May 6, 1995
Reyna, Ignacio Javier Maria *J.M. Wiest*	Brownian Dynamics of Dilute Semirigid Chains	PhD
Thomas, Seqwana N. *W.N. Delgass and G.T. Tsao*	Hydrolysis of Celloboise: Kinetic Study Study of Various Solid Acid Catalyzed Reaction	MS May 6, 1995
Tolia, Anish *C.G. Takoudis and M.J. Weaver* (Chemistry)	Raman Spectroscopic Characterization of TRansition Metal Films in Heterogeneous Catalytic Reactors	PhD May 6, 1995
Varner, Jeffrey David *D. Ramkrishna and A.E. Konopka* (Biological Science)	Analysis of the Dynamic Behavior of Phenanthrene Degradation	MS May 6, 1995
Wisnewski, Philip A. *F.J. Doyle, III*	Model Reduction, State Estimation and Control for the Cook Zone of a Kamyr Digester	MS May 6, 1995

Course Offerings and Seminars 1993-1994

Course Offering - Fall 1994

Class	Course Title	Instructor	Enrollment
201,301,401	Co-op Seminar	Squires	137
205	Chem. Engr. Calculations	Kessler	128
211	Chem. Engr. Thermodynamics	Squires	124
306	Design of Staged Separation	Wang	142
320	Statistical Modeling & Quality En.	Venkatasubramanian	126
348	Chem. Reaction Engineering	Peppas	63
377	Momentum Transfer	Greenkorn	172
378	Heat and Mass Transfer	Andersen	82
434	Chem. Engr. Laboratory I	Emery, Eckert Houze, Jin	137
456	Process Dyanmics & Control	Doyle	201
461	Biomedical Engineering	Hannemann	42
496	Chem. Engr. Honors Lab	Delgass	33
540	Transport Phenomena	Wiest	34
544	Structure and Prop. of Poly. Mat.	Lackritz	41
597H	Chem. Engineering Honors	Peppas	16
597M	Chemical Engr. Materials Research	Lackritz	7
597T	Biochemical Engineering	Tsao	127
610	Advanced Chem. Engr. Thermo	Talbot	25
620	Transport Phenomena I	Caruthers	11
630	Applied Math. for Chem. Engr.	Pekny	27
668	Colloid Interfacial Phenomena	Franses	14
684	Adv. Computer Aided Process Des.	Reklaitis	8
697A	Nanostructured Materials	Andres	6

Special Projects:

411	Chem. Engr. Science. Research Projects	18
412	Chem. Engr. Design. Research Projects	17
498	Research in Chemical Engineering I	36

Course Offering - Spring 1995

Class	Course Title	Instructor	Enrollment
201,301	Co-op Seminar	Squires	92
205	Chem. Engr. Calculations	Wiest	102
211	Intro. to Chem. Engr Thermo.	Squires	113
306	Design of Staged Separation	Andres	87
320	Statistical Modeling & Qual. Enhan.	Venkatasubramanian	121
348	Chem. Reaction Engineering	Tsao	159
377	Momentum Transfer	Greenkorn	79
378	Heat and Mass Transfer	Kessler	142
430	Principles of Molecular Engr.	Lackritz	197
435	Chem. Engr. Laboratory I	Emery, Eckert Squires, Talbot	156
442	Chemistry and Engr. of High Poly.	Caruthers	71
450	Design and Anal. of Proc. Systems	Pekny	192
510	Intermediate Chemical Engr. Thermodynamics	Franses	16
543	Polymer Reaction Engineering	Peppas	23
597C	Polymer Science Engr. Lab.	Caruthers	3
597D	Interm Process Control	Doyle	71
597H	Chem. Engineering Honors	Peppas	9
621	Transport Phenomena II	Ramkrishna	19
624	Mass Transfer	Sevick/ Muraca	16
660	Chemical Reaction Engineering	Takoudis	22
662	Catalysis	Delgass	10

Special Projects:

411	Chem. Engr. Science Research Project	21
412	Chem. Engr. Design Research Project	8
499	Research in Chemical Engineering II	34

Seminars - Fall 1994

Speaker	Title	Date
Professor Michael T. Klein Chemical Engineering Department University of Delaware Newark, DE 19716	Chemical Modelling of Structures, Reactivity and Reaction in the Study of Complex Mixtures	September 15
Dr. Bryan Ennis Agricultural Products & Corporate Center for Particle Science & Tech. E.I. duPont de Nemours & Company Wilmington, DE 19880	Aspects of the Physical Modeling and Control of Granulation Processes	September 22
Dr. Jeffrey J. Siirola Research Laboratories Eastman Chemical Company Kingsport, TN 37662	An Industrial Perspective on Process Synthesis	September 29
Professor Michael J. Betenbaugh Department of Chemical Engineering Johns Hopkins University Baltimore, MD 21218-2694	Engineering the Assembly Pathway in Insect Cells	October 6
Dr. Lowell B. Koppel SETPOINT, INC. 950 Threadneedle, Suite 200 Houston, TX 77079	Economic Benefits of Information Systems in Process Industries	October 13
Dr. Bruno Notari Notari Tecnologie Milan, Italy	Microporous Titanium Silicates	October 20
Professor Dinesh O. Shah Chemical Engineering Department University of Florida Gainesville, FL 32611-2022	Horizons in Surface Science: From Microemulsions to Nanoparticles	October 27
Dr. Osman Basaran Chemical Technical Division Oak Ridge National Laboratory Oak Ridge, TN 37831-6224	Dynamics of Drops and Bubbles: Fluid Dynamics, Interfacial Phenomena, and Effects of Electric Fields	November 3
Professor Yannis Kevrekidis Chemical Engineering Department Princeton University Princeton, NJ 08544-5263	Catalysis on Microstructured Surfaces	November 10
Professor Douglas S. Clark Chemical Engineering Department University of California Berkeley, CA 94720-9989	Taking Biotechnology to Extremes: New Opportunities for Extremophiles	December 1

Seminars - Fall 1994 (continued)

Speaker	Title	Date
Professor Gianni Astarita Chemical Engineering Department University of Delaware Newark, DE 19716	Micromixing and Memory in Chemical Reactors	December 6
Professor Andrew Hrymak Chemical Engineering Department McMaster University Hamilton, Ontario, Canada L8S 4L7	3-D Simulation of Multilayer Polymer Flows	December 8

Seminars - Spring 1995

Speaker	Title	Date
Professor Ignacio Grossmann Department of Chemical Engineering Carnegie-Mellon University Pittsburgh, PA 15213	**Recent Advances in Mixed-Integer** Nonlinear Programming Techniques for the Optimization of Process Systems	**January 26, 1995**
Professor Julia A. Kornfield Chemical Engineering Department California Institute of Technology Pasadena, CA 91125	The Dynamics of Block Copolymer Nanostructures	February 9, 1995
Professor George Georgiou Chemical Engineering Department The University of Texas at Austin Austin, TX 78712-1062	Protein Production In Bacteria	February 23, 1995
Professor Matthew V. Tirrell Chemical Engineering & Materials Science Department University of Minnesota 421 Washington Avenue SE Minneapolis, MN 55455	Shear-Induced Orientation of Diblock Copolymers	March 2, 1995
Professor Julio Ottino Dept. of Chemical Engineering Northwestern University Evanston, IL 60208	Modelling of Mixing Processes: Fluids, Particulates and Powders	March 23, 1995
Professor K.D. Wittrup Chemical Engineering Department University of Illinois Urbana, IL 61801	Engineering Yeast for Enhanced Secretion of Pharmaceutical Proteins	March 30, 1995
Professor Douglas Lauffenberger Department of Chemical Engineering Massachusetts Institute of Technology Cambridge, MA 02139	Engineering Receptor-Mediated Cell Functions	April 6, 1995 Kelly Lecturer
Professor John A. Quinn Chemical Engineering Department University of Pennsylvania Philadelphia, PA 19104-6393	The Motility of Swimming Bacteria: Observation and Simulation	April 13, 1995
Dr. John Monnier Eastman Chemical Company P.O. Box 1972 Kingsport, TN 37662	Selective Epoxidation of Non-allylic Olefins over Supported Silver Catalysts	April 20, 1995