The School of Chemical Engineering

Annual Report

July 1, 1995-June 30, 1996

Purdue University
West Lafayette, Indiana

Frank Oreovicz, editor; Carolyn Blue, compiler

Pamela Burroff-Murr, designer; Ruth Davis, production assistant
Engineering Productions Office

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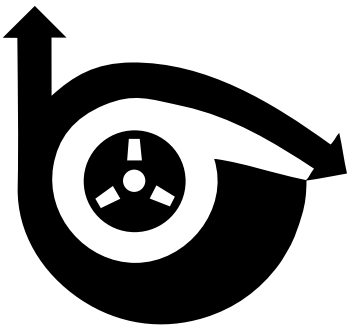
Academic Year Highlights



1995-1996

Academic Year Highlights

The School of Chemical Engineering

Faculty Affairs

Faculty Appointments

In July 1995, Professor Osman Basaran joined the School, after appointments as group leader in the Chemical Technology Division of Oak Ridge National Laboratory and as senior research engineer with Air Products & Chemicals. Professor Basaran's research 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, especially high speed visualization of drop formation and impact. His BS ChE is from MIT (1978) and PhD was awarded at the University of Minnesota (1984). In Spring 1996, he taught a well received graduate course on Finite Element Analysis in Chemical Engineering and in Fall 1996 will teach the core graduate course on Transport Phenomena.

During the year, the School attracted to our faculty Dr. Jochen Lauterbach, who will commence his appointment in August 1996 with the rank of Assistant Professor. A native of Germany, Dr. Lauterbach graduated from the University of Bayreuth with a Diploma in Technical Physics and completed PhD studies at the Free University of Berlin in 1994. His doctoral research at the Fritz Haber Institute was directed by Prof. G. Ertl, who is generally acknowledged to be one of the world's foremost experts in surface science and heterogeneous catalysis. In November 1994, Lauterbach was granted the Feodor Lynen Fellowship of the Humboldt Foundation, a highly competitive postdoctoral award, and has been working with Prof. W.H. Weinberg at the University of California, Santa Barbara, on the characterization of nonlinear phenomena which occur during surface reactions. Dr. Lauterbach is a very highly regarded experimentalist, skilled in a range of spectroscopic techniques, and a very productive researcher, with some 20 publications to his credit to date. He will be actively involved in developing and teaching experimentally oriented courses at the dual and graduate levels.

With the enthusiastic support of the faculty, Professor W. Nicholas Delgass was named to the position of Associate Head of the School, effective with the 1995-96 fiscal year. Professor Delgass, a member of the faculty since 1974, has had broad experience in all aspects of academic research, teaching, and service. He maintains an active program of research in heterogeneous catalysis, has championed the creation of the Dow Advanced Instrumentation Laboratory and associated course, has served on a number of key University, Engineering, and School committees, including all levels of the promotion process, and also is

Editor of the Journal of Catalysis. He was instrumental in helping to launch the New Directions in Chemical Engineering program and has served on the Faculty Advisory Committee for the program since its inception. As Associate Head, he has responsibility for academic program administration, including course planning and staffing and scholarships, and for Undergraduate Studies Office.

Additional faculty appointments this year included the advancement of Profs. Hilary Lackritz and Eva Sevick-Muraca to the rank of Associate Professor of Chemical Engineering with Tenure, effective August 1996. Professor Lackritz has served on the faculty since Fall 1991 and Professor Sevick-Muraca since Fall 1994. Professor Julian Talbot left the faculty at the end of the academic year to pursue other career interests. During the 1995-96 academic year, Professor George Tsao was on sabbatical leave as Visiting Professor of Chemical Engineering at the Hong Kong University of Science and Technology. Beginning in January 1996, Professor Joe Pekny took leave for a year to collaborate with several major corporations in the development and application of combinatorial optimization methods for batch process design, scheduling, and supply chain management problems.

For the fall 1995 semester, the School appointed Donald Hannemann to the position of Shreve Visiting Industry Professor. Mr. Hannemann, who recently retired after a very productive career as senior research manager with Amoco Corporation, was instrumental in organizing and team teaching with the faculty a new course, CHE 597B, The Chemical Process Industry. The course, which drew nearly 80 registrants, provided an overview of the structure of the industry, the main chemical building blocks, and the chemical technology network which the products of the industry constitute. In Spring 1996, Dr. Cristi Bell-Huff joined the School as Visiting Assistant Professor. Dr. Bell received her BS ChE from the University of Tennessee and PhD from Purdue, working with Professor Nicholas Peppas. She returned to Purdue after two years with Hoechst-Celanese as R&D engineer in the polymer area. She very ably taught the polymer elective course, ChE 442, and was part of the faculty team teaching the senior laboratory course, CHE 435. Dr.Bell-Huff terminated her appointment in May to accept another position. Finally, during the 1996-97 academic year, Dr. Balaji Narasimhan, has been appointed Visiting Assistant Professor in the School. Dr. Narasimhan received his B.Tech. in ChE at IIT Bombay in 1992 and PhD in 1996 from our School, working with Professor Peppas. He has served as visiting researcher under Prof. Gianni Astarita, University of Naples; Prof. Sir Sam Edwards, University of Cambridge,; and Prof. Bob Langer, MIT. His research interests lie in diffusion in polymers, polymer dissolution, dynamics of polymer motion, and molecular modeling. In the Fall semester, he will be team-teaching the polymer physics elective, ChE 544, with Professor Lackritz and, in addition, will be involved with the senior lab course, ChE 434.

Professor Robert Greenkorn, Slayter Distinguished Professor of Engineering, who serves as Special Assistant to the President and Vice President of the Purdue Research Foundation, was appointed to the additional position of Director of the Purdue Technical Assistance Program. In January 1996, Professor Philip Wankat resigned from the post of Head of Freshman Engineering and accepted the transitional

assignment of Interim Director of the Continuing Engineering Education program. In January 1997, he will return to full-time professorial duties in the School of Chemical Engineering.

Professional Recognition

In July 1995, Professor Sevick-Muraca received a National Institutes of Health Research Career Development Award, a very prestigious five year award which allows her to advance her research in optical imaging and spectroscopy in the field of biomedical engineering. She joins a very small and distinguished group of chemical engineering researchers in the bioengineering domain who have been recognized by this award over the years. In Spring of this year, Professor Doyle was named recipient of the Office of Naval Research Young Investigator Award. This three year award is directed towards advancing his research on approaches to nonlinear process control through neuromimetics. He was also winner of the 1966 ASEE Illinois / Indiana Section Outstanding Teaching Award, the 1996 Tau Beta Pi Dean Marion B. Scott Exemplary Character Award, and was one of the Schools of Engineering nominees for the University-wide 1996 Murphy Undergraduate Teaching Excellence Award.

Professor Ramkrishna was named a Fellow of the American Institute for Medical and Biological Engineering, joining Profs. Peppas and Tsao who had achieved this distinction in prior years. The induction took place at the March meeting of the AIMBE in Washington DC. Professor Robert Squires was winner of the 1996 Shreve Outstanding Teaching Award of the School. This is the sixth time that Professor Squires has won this award in the past twenty years.

Several of the faculty accepted new editorial appointments in the past year. Professor Lackritz was invited to be Guest Editor of the Journal of Polymer Science : Polymer Physics 1997 special issue, serving on behalf of the Division of High Polymer Physics of the American Physical Society. Professor Sevick-Muraca was invited to be Special Topics Editor for *Applied Optics* 1966 special issue on fluorescence diagnostics in tissues and the *Journal of the Optical Society of America A* 1996 special issue on fluorescence dynamics for diagnostics. Professor Venkatasubramanian was named to the Editorial Board of *Process Safety Progress.* Professor Wankat was appointed Associate Editor of *Chemical Engineering Education* and continues as Editor-in-Chief of *Separation and Purification Methods*.

Professional Activities

The expertise of the faculty is being recognized through a growing number of appointments to professional society committees, panels, and boards. Together with colleagues from the California Institute of Technology and the University of Texas, Professor Andres serves on the organizing committee of the 1996 Joint Japan-US Workshop on Nanoparticle Synthesis and Applications which will be held in Tsukuba, Japan, in October, 1996 under the joint sponsorship of the JSPS and the NSF. Professor Basaran was invited to participate in the Discontinuous Coating Workshop convened at the NSF Center on Interfacial Engineering, at the University of Minnesota (May, 1996) and served on the steering committee for the NSF-EPRI Workshop on Electroseparations. Professor Doyle was invited participant at the NSF Workshop on Architecture for Control and Learning in Natural and Artificial Systems held in November. Professor Hannemann was

elected Vice President (and President-elect) of the American Academy of Pediatrics. Professor Peppas was selected to the External Affairs Committee of the Materials Research Society, to the Fellows Committee of the Society for Biomaterials, and served on the NSF Panel of Technology for a Sustainable Environment. During December, Professor Ramkrishna was World Bank Visiting Professor at several universities in the Peoples Republic of China. Professor Sevick-Muraca was appointed to the Advisory Board for the Laboratory for Fluorescence Dynamics at the University of Illinois, Urbana-Champaign, and served on the NSF review panel of Optical Science and Engineering and the NIH panel on Resource Research Review. Professor Venkatasubramanian was appointed to the New Technology Task force of the AIChE. Professor Wang was named to the ACS Canvassing Committee for the Separations Award. Professor Wankat was appointed to the AIChE Award for Service to Society Subcommittee.

The faculty was involved in leading roles in the planning and organization of international conferences. Professor Doyle was invited to the Programming Committee for ADCHEM 97, an international specialist conference on advanced chemical process control, and PSE 97/ESCAPE 97, the sixth in an international triennial series on Process Systems Engineering. Professor Franses served on the International Advisory Committee of the International Symposium on Micelles, Microemulsions, and Monolayers convened in August. Professor Lackritz served as ACS Polymer Chemistry Division Program Co-chair for the 1995 joint meeting with OSA as well as for the 1996 Orlando meeting. Professor Peppas was invited to the Scientific Advisory Board of the First Spanish-Portuguese Conference on Controlled Drug Delivery held in September and serves on the Organizing Committees for the Seventh International Symposium on Drug Delivery, and the Materials Research Society San Francisco Meeting. Professor Reklaitis chaired the CCR-NSF Workshop on World-wide Industry-University-Government Research Collaboration Models in the Chemical Sciences and Engineering held in October. Professor Sevick-Muraca is program chair for the Optical Society of America 1996 Topical Meeting for Biomedical Optical Spectroscopy and Diagnostics. Professor Venkatasubramanian co-chaired the International Conference on Intelligent Systems in Process Engineering convened in July and was also appointed to the International Program Committee of PSE'97/ESCAPE 7. Professor Wang is member of the Organizing Committee for the 1996 International Symposium on Preparative Chromatography.

Collectively, the faculty served as chairs, organizers, or members of advisory committees for over thirty-five conferences and symposia. Professor Basaran chaired the first-ever session on Atomization Coating in the 8th Biennial Coating Symposium held in conjunction with the AICHE Spring Meeting. Professor Doyle chaired the session on Robust Control of Linear Systems at the European Control Conference held in Italy in September. Professor Lackritz chaired the session on Polymer Relaxation Dynamics at the American Physical Society meeting in St. Louis. Professor Peppas chaired a block of sessions on Diffusion in Polymers, Professor Ramkrishna a session on Stochastic Methods, and Professor Sevick-Muraca a session on Optical Techniques in ChE at the AICHE Annual Meeting. Professor Reklaitis chaired the plenary session on Globalization of Research at the Council for Chemical Re-

search Annual Meeting. Professor Sevick-Muraca organized and chaired the session on New Directions for Time-Dependent Measurements of Photon Migration at the Engineering Foundation Conference on Lasers in Medicine and Surgery. Professor Venkatasubramanian was chair of the session on Computer Integrated Manufacturing in the Process Industries jointly sponsored with the Japan Society of Chemical Engineers at the AIChE Annual Meeting.

The faculty continue to be very active on the lecture and seminar circuit, collectively giving some 80 invited lectures at conferences and academic and industrial sites. Professor Andres addressed the International Symposium on the Sciences and Technology of Atomically Engineered Materials. Professor Basaran was plenary lecturer at the NSF-EPRI Workshop on Electroseparations. Professor Caruthers gave invited lectures at the MRS Annual Meeting and at the March APS meeting. Professor Doyle was invited lecturer at Chemical Process Control V, a prestigious conference held only once every five years. Professor Lackritz lectured at the International Conference on Advanced Materials of the IUMRS held in Mexico. During May, Professor Peppas gave a series of lectures as Visiting Professor at the University of Naples, Italy. Professor Ramkrishna was plenary lecturer at Chemcon 95, a joint meeting of AICHE and IIChE held in India. Professor Reklaitis presented an invited lecture at the International Symposium on Intelligent Systems in Process Engineering. Professor Sevick-Muraca was invited lecturer at the NATO Workshop on Analytical Use of Fluorescent Probes in Oncology and the Laser Focus World's Medical Laser Marketplace seminar. Professor Wang lectured at the 26th Annual Meeting of the Fine Particle Society. Professor Venkatasubramanian presented seminars at Imperial College, Loughborough Institute of Technology, ICI Engineering, and the University of Edinburgh.

Staff Affairs

In January of this year, Mrs. Phyllis Beck, who had voluntarily reduced her secretarial appointment to half time earlier, retired from the University after nearly 40 years of loyal service to Purdue University. In March 1996, Ms. Suzanne S. Flavin joined the staff of the School as Secretary IV, after many years of experience in various university offices, most recently the Office of the Vice President for Student Affairs. She replaced Ms. Kim Trethewey who left to pursue other interests. In the following month, Ms. Anne Hardie Davidson joined the Business Office of the School as purchasing clerk. A recent graduate of the Purdue School of Liberal Arts, she took on duties previously held by Mrs. Kamela Lawrence, who was appointed payroll clerk, a position previously held by Tonya Reid. Ms. Reid was promoted and transferred to another business office in Engineering. As a result of these changes, at the close of the fiscal year, the secretarial staff of the School consisted of 6.5 FTE plus one vacancy, while the Business Office consisted of Ms. Hannah Moore plus two clerical staff.

Graduate Education and Research

Research Productivity

The research productivity of the faculty as measured by expenditures, proposal activity, publications and conference presentations has remained sustained at high levels. Total research expenditure, including funds from federal, industrial and unrestricted sources, was at the level of $4.76 million, an increase of 10% from the previous year. Indeed, expenditures of external funds continue to dominate expenditures of internally budgeted University general funds by a considerable margin. In 1995-96 University general funds constituted 35.2% of the total expenditures of the School. This percentage has been steadily declining from the level of 44.7% in 1990-91, reflecting the flat profile of University general funds and strong growth of external funds over the past six years. These totals exclude the separately budgeted expenditures of the Laboratory for Renewable Resources Engineering, directed by Professor Tsao. This level of research funding was sustained by significant proposal writing efforts of the faculty. Over the past year, dollar volume of new proposals increased by 16% from the previous year to a level of $15 million and awards increased by 6.5% to $3.03 million. Unrestricted grants, gift funds, and gifts in kind held level at $1.27 million.

The tangible results of the intense research effort of the faculty and research staff included over 275 refereed papers in various stages of the publication process, an increase from the 230 reported in the previous year. The research groups contributed 132 conference presentations, compared to 120 reported in the previous year. When combined with the 80 invited lectures and seminars, this total translates to an average of about 11 lectures / presentations per active research faculty member per year. Given the very high enrollments which the School has sustained over the past several years with the attendant high teaching and mentoring demands, the level of research and professional activity of the faculty is exemplary.

Graduate Program

Fall 1995 enrollments declined modestly by admission control from the 128 of the previous year to 117. The School graduated 20 PhD and 13 MS students in 1995-96 compared to 21 PhD and 20 MS in the previous year. Of the 13 MS graduates, six continued towards the PhD. The School's PhD graduation rates are likely to continue to position Purdue ChE among the top 5 PhD granting ChE departments in the country: last year we were 3rd. In Fall 1996 the School expects to admit 20 new graduate students, 8 of whom are international students, 2 minority, and 6 women. By contrast, 24 students were admitted in Fall 1995 and two additional students were admitted in January, 1996. Employment prospects for advanced degree candidates is improving: of the 20 PhD and 7 terminal MS students graduating this year, only one had not found employment by the time of thesis defense.

The Graduate Student Organization of the School convened the fourth annual Chemical Engineering Graduate Research Symposium on August 17, 1995. The program featured formal presentations by 25 senior graduate students in two parallel sessions as well as poster presentations by 14 junior graduate students. Fourteen companies were represented and these representatives served as the jury for the selection of the best presentations. The winners were as follows:

	Session 1	Session 2
First place	M. Bassett	C. Hutchinson B. Maner
Second Place:	J. Bielefeld R. Ramkrishna	C. Brazel C. Panczyk

The chair of the symposium was Ted Pirog. The Fifth Annual Symposium is scheduled to take place on August 15, 1996 and will be chaired by Chris Williams.

Instruction

Awards

The high quality of the instructional programs of the School is the result of the combined efforts of the faculty, the teaching assistants, and the support staff. The fine contributions of the teaching assistants were recognized through the 1996 Purdue University Magoon Awards which were presented to Jeffrey Varner and Steven Honkomp. Theodore Pirog was selected by the seniors for the Award for Teaching Excellence in the Undergraduate Laboratory.

The 1996 student awards voted by the faculty and presented at the awards banquet were as follows: The Junior awards were designated for Jeffrey E. Lin, Steven Craig Award, and Andrew C. Allock, the George T. Tsao Award. Among the seniors, Krista M. Fitzsimmons won the AICHE Outstanding Senior Award, Craig Beasley the Omega Chi Epsilon Award, Karleen L. King, the Lottes Award, and Jennifer E. Harting, the American Institute of Chemists Award. The annual Senior Design Project Award, given to the student team that produces the best design for the longer term case study executed in the senior process design course, was won by the design group of Jennifer Harting, Lisa LaMacchia, and John Willham. In second place was the team of Craig Beasley, Matthew Colburn, and Douglas Heintzelman.

Enrollment Trends

The Fall 1995 undergraduate enrollment of the School was 610, a decline from the previous year's historical high of 676. The decline occurred as a result of the second year of imposition of a 2.9/4.0 grade point based cap on transfers of students who had completed the Freshman Engineering program. This year the School also experienced its largest ever graduating class totaling 186 students over the August, December, and May graduations. This is a slight increase from the 185 of the previous year. These graduation rates certainly sustain the position of this School as the number one ChE program in terms of number of BS graduates. In Fall 1996 we expect enrollments to decline by about 100 students, bringing enrollments more in line with long term goals for the School.

The employment prospects for the 1996 class continued to improve over previous years, with some 25% of the class with unknown employment status at the time of graduation. The May graduating class consisted of 165 students, 39% women, and 26% students who had completed the cooperative education program. Only 5% of the coops had no firm job commitments at the time of graduation.

Honors and Undergraduate Research Programs

The faculty has maintained a high level of commitment for providing undergraduate students with research and extended duration independent project experiences. In 1995-96, 16 students seniors completed the Honors BS program, compared with 34 in the previous year. The decline is a direct result of a review and revision of the program which was undertaken in Spring 1995 to tighten the qualifying grade point average, the progress reporting requirements, and the formal course requirements. At present the Honors program requires a minimum GPA of 3.6, grades of B or better in seven core courses, a one year bachelor's thesis research project, a more challenging senior laboratory course, and an advanced level elective course.

Summer 1995 marked the last year of the NSF Research Experience for Undergraduates grant which the faculty had been successful in receiving. A total of 13 students performed research with the faculty under stipends provided by the NSF. In Summer 1996 this activity was replaced by for-credit research projects in which 17 students participated. Over this academic year a total of 95 one semester undergraduate independent research projects were directed by the faculty. This is a significant increase over the 60 of the previous year. These projects involve undergraduates working with graduate students and faculty on specific research projects and thus facilitating one-on-one student-faculty contact. When combined with the Honors projects, which are of two semester duration, in 1995-96, the faculty directed a total of 127 one semester projects, an average of three projects per semester per active research faculty. 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 undergraduate students.

Accreditation

In November of this year, the Schools of Engineering were visited by an ABET team for a review of the various undergraduate programs. As a result, the School of Chemical Engineering was fully accredited for another six year term. The principal suggestions for improvement included reductions in the high student to faculty ratio by the expansion of the faculty, expansion of facilities, including computer resources, to accommodate the large student enrollment, closer coordination between upper and lower division courses, and enhancements to the student mentoring program. The faculty of the School were viewed to be strong and the morale high, in spite of high enrollments. The industrial interaction and support of the School were viewed to be a strength, and the appointment of a Lab Director with extensive industrial experience to be a positive feature of the lab experience of students.

Facilities Development

The renovation of the Dow Advanced Instrumentation and the Polymer Engineering Laboratories was completed in Summer 1995 and the associated laboratory courses offered in Spring 1996. Renovation of Professor Basaran's fluid mechanics laboratory was completed in Spring 1996. The installation of a new climate control system for a

suite of laboratories on the second and third floors was slated for completion in late Summer 1996. Climate control and office and hallway renovation for the first floor suite of offices, including the Main Office, Undergraduate Studies Office, Business Office, the Head's and Associate Head's offices, and several faculty and staff offices were approved by Executive Vice President Ford in Summer 1995. The work was scheduled to begin in August and to be completed by the end of October, 1996. The Dean approved the move of the Interdisciplinary Engineering Program from the CHME Building to the CIVL Building in Spring 1996. This move, which is to be completed in August 1996, will release additional graduate student office space to the School.

During this academic year the Facilities Committee, chaired by Professor Franses, working closely with Dr. Wayne Muench, conducted a detailed audit of the inventory of experiments in the Undergraduate Laboratory and identified experiments which must be retired, those that need to be revamped, as well as opportunities for the introduction of new experiments. As the second step of this study, a detailed renovation plan was developed under which the 4500 sq. ft laboratory would be extensively refurbished, a loft added to the high bay area, and hoods, benches, and cabinets replaced. Because of lack of remaining funds in the 1995-97 biennium budget, the four phase plan was scheduled to begin in Summer 1996 at a modest level with removal of unused utilities lines and other inactive plumbing, painting and patching of walls, and improvements in several key experiments. The entire four phase plan is to be completed by Summer 2000 at a total cost of $1 million, exclusive of new experiments.

Industrial and Alumni Relations

The New Directions in Chemical Engineering partnership program with industry continues to be an active and positive force for the School. The Industrial Advisory Council, which includes representation from 20 major chemical process industry corporations, met in annual meeting on September 22-23, 1995 to review the status of the School, receive a progress report of the accomplishments attained over the past three years of the program, to review the laboratory development plans, and to discuss the needs of the industry in the education and training of chemical engineers. With the retirement of Tom Storer of DuPont from the Executive Committee of New Directions, Deborah Grubbe was elected to membership. Ms.Grubbe, a ChE graduate of Purdue, is Director, Engineering of DuPont. The Executive Committee, consisting of eight senior CPI executives, met on February 26-27 at Amoco offices in Houston and June 26-27 at DuPont offices in Wilmington DE. The items of discussion for the February meeting included a review of the New Directions progress report to be submitted to the membership, discussion of CHME building projects, and evaluation of the previous five year strategic plan of the School. The main agenda items for the June meeting were a discussion of an early draft of the new strategic plan, the review of the agenda for the annual meeting, and discussion of a proposed Minority Scholars Program for which industrial sponsorship will be sought. The next meeting of the Industrial Advisory Council is scheduled to September 20-21, 1996. The focus of the meeting is a thorough discussion of the next draft of the strategic plan.

Alumni Awards

At the May commencement, Dr. Michael Ramage was awarded the Honorary Doctorate in Engineering. Dr. Ramage, (BS'66, MS'69, and PhD'72) is President of Mobil Technology Company and Chief Technical Officer of Mobil Corporation. He was honored for an outstanding career in research and research management. Earlier in the Spring, two ChE alumni were awarded Distinguished Engineering Alumnus Awards during the annual DEA Convocation which takes place Gala Weekend. These awardees were Dr. Ching-Tien Liou (MS'71, PhD'72), President of Taiwan Institute of Technology, and Dr. David Rea (BS'62), Vice President of DuPont Central Research.

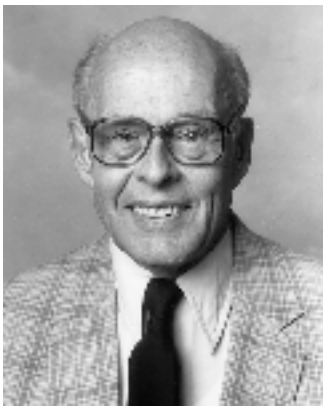
Three alumni were selected to receive 1995 Outstanding Chemical Engineer Awards: Robert Buckman (BS'59) President and CEO of BULAB Holdings and Vice Chair of the Board of Buckman Laboratories; Thomas Storer (BS'59) Director, DuPont Human Resources; and Dr. Sarah M. Willoughby (PhD'50) Prof. Emerita, Texas A&M. Among many other distinctions, Dr. Willoughby is the first woman PhD of the Schools of Engineering. These awards were presented during the course of individual visits to the campus which included seminars which the recipients gave to the 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

Kinetics and Processes of Organic Reactions (especially pyrolysis, alkylation of isobutane, nitration, and hydrogenation of vegetable oils)

High polymers and Polymerization

Gasification and Liquefaction of Coal

Paper Production

Publications

am Ende, D.J., Eckert, R.E. and Albright, L.F., "Interfacial Area of Dispersions of Sulfuric Acid and Hydrocarbons," *Ind. Eng. Chem. Research* 34, 4343, 1995.

Albright, L.F., "Nitration," Kirk-Othmer Encyclopedia of Chemical Technology, 4th Edition, Vol. 17, 68-80, 1996.

Albright, L.F. and Lang, E.G., "Sulfuric Acid Recovery from Alkylation Units and Other Processes," Encyclopedia of Chemical Processing and Design, J.J. McKetta (ed.), Vol. 55, pp 456-468, Marcel Dekker, Inc., New York, 1996.

Albright, L.F., Carr, R.V.C. and Schmitt, R.J., editors, Nitration: Recent Laboratory and Industrial Developments," ACS Symposium Series #623, American Chemical Society, Washington, DC, 1996.

Albright, L.F., Sood, M.K. and Eckert, R.E., "Modeling NO_2+ Concentrations in HNO_3-H_2SO4-Water Mixtures," ACS Symposium Series #623, pp 201-213, American Chemical Society, Washington, DC, 1996.

Editorial Boards

Encyclopedia of Chemical Processing and Design (1976-present)

Polymer News (1995-present)

Invited Lectures

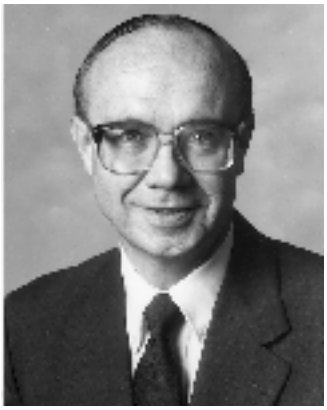
Nine chapters of American Institute of Chemical Engineers.

** Year of joining the faculty.*

Ronald P. Andres

1981

Engineering Research Professor



Degrees

BS, Northwestern University, 1959

PhD, Princeton University, 1962

Interests

Ultrafine Particles

Nanostructured Materials

Nanoelectronic Devices

Catalysis

Research Areas

Electronic Conduction in Molecular Nanostructures: The development of MBE 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 lateral superlattices by interconnecting metal clusters, that have uniform diameters in the 1 - 10 nm size range, by means of organic molecules. These linked cluster arrays exhibit a wide variety of interesting electronic behavior including exciting new quantum effects.

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 physical properties. 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: (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 se-

ries 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 developing 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 exponentialy and the atomic configuration or structure of the cluster becomes important. Furthermore, even if clusters with desirable physical or chemical properties can be synthesized in the gas phase, one must devise practical processes by which these ultrafine particles can be assembled to produce a film or a 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. We have synthesized several novel catalytic and optoelectronic materials in this way.

Publications

Schaefer, D.M., R. Reifenberger, A. Patil and R.P. Andres, "Fabrication of Two-Dimensional Arrays of Nanometer-Size Clusters with the Atomic Force Microscope," *Appl. Phys. Lett.*, *66*, 1012, 1995.

Schaefer, D.M., A. Patil, R.P. Andres and R. Reifenberger, "Elastic Properties of Individual Nanometer-Size Supported Gold Clusters," *Phys. Rev. B.*, *51*, 5322, 1995.

Dorogi, M., J. Gomez, R. Osifchin, R.P. Andres and R. Reifenberger, "Room-Temperature Coulomb Blockade from a Self-Assembled Molecular Nanostructure," *Phys. Rev. B*, *52*, 9071, 1995.

Andres, R.P., "Inelastic Energy Transfer in Particle/Surface Collisions," *Aerosol Sci, & Tech.*, *23*, 40-50, 1995.

Mahoney, W., S.T. Lin and R.P. Andres, "Probing the Nucleation of a Thin Metal Film: Atom Deposition vs. Cluster Beam Deposition," *Mat. Res. Soc. Symp. Proc.*, *355*, 83, 1995.

Bielefeld, J.D., R.G. Osifchin and R.P. Andres, "A Comparison of the Physical Properties of Cluster-Based and Vacuum-Evaporated Thin Metal Films," *Mat. Res. Soc. Symp. Proc.*, *355*, 359, 1995.

Osifchin, R.G., W.J. Mahoney, J.D. Bielefeld, R.P. Andres, J.I. Henderson and C.P. Kubiak, "Synthesis of a Quantum Dot Superlattice Using Molecularly Linked Metal Clusters," *Superlattices and Microstructures*, *18*, 283, 1995.

Janes, D.B., V.R. Kulagunta, R.G. Osifchin, J.D. Bielefeld, R.P. Andres, J.I. Henderson and C.P. Kubiak, "Electronic Conduction Through 2D Arrays of Nanometer Diameter Metal Clusters," *Superlattices and Microstructures*, *18*, 276, 1995.

Mahoney, W. and R.P. Andres, "Aerosol Synthesis of Nanoscale Clusters Using Atmospheric Arc Evaporation," *Materials Science & Engineering, A260*, 160, 1995.

Andres, R.P., T. Bein, M. Dorogi, S. Feng, J.I. Henderson, C.P. Kubiak, W. Mahoney, R.G. Osifchin and R. Reifenberger, "Coulomb Staircase at Room Temperature in a Self-Assembled Molecular Nanostructure," *Science, 272*, 1323, 1996.

Andres, R.P., S. Datta, M. Dorogi, J. Gomez, J.I. Henderson, D.B. Janes, V.R. Kolagunta, C.P. Kubiak, W. Mahoney, R.G. Osifchin, R. Reifenberger, M.P. Samanta and W. Tian, "Room Temperature Coulomb Blockade and Coulomb Staircase from Self-Assembled Nanostructures," *J. Vac. Sci. Technol. A, 14*, 1178, 1996.

Meeting Presentations

"Synthesis of Quantum Dot Superlattices Using Molecularly Linked Metal Clusters," Eighth International Conference on Superlattices, Microstructures, and Microdevices, Cincinnati, OH, August 1995.

"Synthesis of Electronically Coupled Superlattices from Nanometer Diameter Metal Clusters," Third International Symposium on Quantum Confinement: Quantum Wires and Dots, Chicago, IL, October 1995.

"Investigation of Neutral Cluster-Beam Deposition as an Alternative Metallization Process," AIChE 1995 Annual Meeting, Miami, FL, November 1995.

"Structure and Elastic Properties of Nanometer-Size Metal Clusters," AIChE 1995 Annual Meeting, Miami, FL, November 1995.

"Highly Dispersed Inverse Mixed Catalysts," AIChE 1995 Annual Meeting, Miami, FL, November 1995.

"Aerosol Synthesis of Nanoscale Ceramic Particles Using Atmospheric Arc Evaporation," AIChE 1995 Annual Meeting, Miami, FL, November 1995.

"Self-Assembly of Two Dimensional Arrays of Metallic Nanoparticles," MRS Meeting, Boston, MA, November 1995.

"Microstructure and Electromigration Properties of Gold Lines Formed by Neutral Cluster Beam Deposition," MRS Meeting, Boston, MA, November 1995.

"Aerosol Synthesis of Metal and Metal Oxide, Nitride, and Carbide Nanoparticles Using an Arc Evaporation Source," MRS Meeting, Boston, MA, November 1995.

"Self-Assembly of a Two-Dimensional Superlattice of Nanometer Diameter Metal Clusters Linked by Organic Molecular Wires", APS March Meeting, St. Louis, MO, 1996.

"Self-Assembly of Two-Dimensional Superlattices of Linked Metal Clusters," Eighth International Symposium on Small Particles and Inorganic Clusters, Copenhagen, Denmark, July 1996.

Invited Lectures

"Fabricating a Linked Cluster Network: A Novel Artificially Engineered Material," Materials Engineering Seminar, Purdue University, January 1996 and Electrical Engineering Seminar, University of Cincinnati, February 1996.

Osman Basaran

1995

Professor

Degrees

BS, Chemical Engineering, MIT, 1978

PhD, Chemical Engineering, University of Minnesota, 1984

Interests

Drop and bubble dynamics, fluid mechanics

Electric, magnetic, and acoustic field-enhanced processing

Interfacial phenomena and dynamic surface tension measurement

Atomization coating and delivery of agricultural chemicals

Computational analysis: finite element, boundary element and VOF methods

Experimental analysis: ultra high-speed visualization and particle sizing

Research Areas

The major theme of the research is to carry out a scientifically based experimental and computational program of study that will lead to improvements in, or discoveries of systems, processes, and products of engineering importance. The work addresses three distinct areas: (1) separations, (2) materials processing, and (3) measurement of interfacial properties. These apparently distinct areas are nevertheless intimately related because a feature that is not only common but central to each is the presence of free boundaries—fluid interfaces—that enclose drops, bubbles, and films.

A second unifying theme of the research is the use of external fields, e.g. electric or acoustic. The three focus areas are: (1) Separations. Separation processes arise in applications as diverse as refining of petroleum and purification of drugs in chemical, petroleum, and pharmaceutical industries.

Separations are also major consumers of energy. Multiphase systems containing drops, bubbles, and films play a central role in determining the behavior of a number of separation processes, e.g. extraction and distillation. However, not only are the transport underpinnings of such systems often delegated to second-class status compared to their thermodynamic behavior but, worse yet, our understanding of important issues concerning flow and mass transfer is based entirely on empiricism. This research aims to develop new and efficient separation processes by remedying our lack of understanding of transport fundamentals on the one hand and employing electric or acoustic fields in novel ways to enhance the dispersion, motion, and coalescence of drops/bubbles on the other hand.

(2) Materials processing. The challenge here is to effectively manipulate liquid drops and fluid interfaces **to exploit to benefit** the interaction between the underlying transport phenomena during processing and the microstructure of the resulting material. A major objective is to explore ways to use to advantage electric and acoustic fields in coating flows, polymer processing, and powder synthesis. Attention is currently focused on a variety of problems including synthesis of ceramic powders by electro-atomization, microencapsulation, blending of polymers, and field-assisted hydrodynamic wetting. A major area of focus is atomization coating (also painting and printing), where the central problem is the impact of one or more drops on a substrate. Recent environmental regulations demand that spray coating industries switch to nonsolvent-based coating liquids or ones having high loadings of polymer and solids. **To date, rational advances** in these applications have been slow because computational analysis of free surface flows of such complex materials **are only in their infancy.** Remedying this situation is a major goal of the research.

(3) Measurement of interfacial rheological properties. In the applications described previously and also in crop spraying, which is yet another area of inquiry in the PI's group, certain physical properties play a dominant role in determining system response. One property of particular interest is dynamic surface tension (DST). Superior techniques are needed compared to ones that currently exist that are capable of making reliable measurements of DST in on the order of milliseconds or faster. Several such techniques are being developed by the PI's group that rely on ultra high-speed visualization and computation based on the finite element method and competing methods for solving free boundary problems.

Awards and Major Appointments

Exxon Education Foundation Award

Publications

Zhang, X., O.A. Basaran and R.M. Wham, "Theoretical prediction of Electric Field-enhanced Coalescence of Spherical Drops," *AIChE J.*, 41, 1629, 1995.

DePaoli, D.W., J.Q. Feng, O.A. Basaran and T.C. Scott, "Hysteresis in Forced Oscillations of Pendant Drops," *Phys. Fluids,* 7, 1181, 1995.

Zhang, X. and O.A. Basaran, "An Experimental Study of Dynamics of Drop Formation," *Phys. Fluids,* 7, 1184, 1995.

Basaran, O.A., T.W. Patzek, R.E. Benner and L.E. Scriven, "Nonlinear Oscillations and Breakup of Conducting, Inviscid Drops in an Externally Applied Electric Field," *I&EC Research,* 34, 3454, 1995.

Franses, E.I., O.A. Basaran and C.-H. Chang, "Techniques to Measure Dynamic Surface Tension," *Current Opinions* ,1, 296, 1996, invited review paper.

Harris, M.T., W.G. Sisson, S.M. Hayes, S.J. Bobrowski and O.A. Basaran, "Porous Spherical Shells and Microspheres by Electrodispersion Precipitation," *Mat. Res. Soc. Symp. Proc.,* 372, 43, 1995.

Wham, R.M., O.A. Basaran and C.H. Byers, "Wall Effects on Flow Past Solid Spheres at Finite Reynolds Number," *I&EC Research,* 35, 864, 1996.

Zhang, X. and O.A. Basaran, "Dynamics of Drop Formation from a Capillary in the Presence of an Electric Field," accepted for publication in *J. Fluid Mech.*, 1996.

Zhang, X. and O.A. Basaran, "Nonlinear Deformation and Breakup of Stretching Liquid Bridges," accepted for publication in *J. Fluid Mech*, 1996.

Patents

Sisson, W.G., M.T. Harris and O.A. Basaran, "Nozzle for electric dispersion reactor," U.S. Patent No. 5,464,195, November 7, 1995.

Harris, M.T., O.A. Basaran, T.G. Kollie and F.J. Weaver, "Silica powders for powder evacuated thermal insulating panel and method," U.S. Patent No. 5,480,696, January 2, 1996.

Basaran, O.A., M.T. Harris, T.C. Scott and W.G. Sisson, "Improved nozzle for electric dispersion reactor," U.S. Patent No. 5,503,372, April 2, 1996.

Invited Lectures

Basaran, O.A., "Drop Dynamics in Electroseparations," departmental seminar, Department of Chemical Engineering, University of Washington, Seattle, WA, April 8, 1996.

Basaran, O.A., "Dynamics of Impact of Complex Liquid Drops with a Substrate: Effects of Surface and Bulk Rheology," Discontinuous Coating Workshop, NSF Center for Interfacial Engineering, University of Minnesota, Minneapolis, MN, May 16, 1996.

Basaran, O.A., "Electric Field-Enhanced Surface Area Generation, Drop Coalescence, and Fluid Convection," NSF-EPRI Workshop Electro-Separations 2020, Arlington, VA, October 9-11, 1995.

Chaired Conferences/ Symposia

Member of the Steering Committee, NSF-EPRI Workshop Electro-Separations 2020, Arlington, VA, October 9-11, 1995.

Meeting Presentations

Basaran, O.A. and E.D. Wilkes, "Forced Oscillations of Supported Drops," Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.

Basaran, O.A. and X. Zhang, "Formation of Conducting Drops in an Electric Field," AIChE Annual Meeting, Miami Beach, CA, November 12-17, 1995.

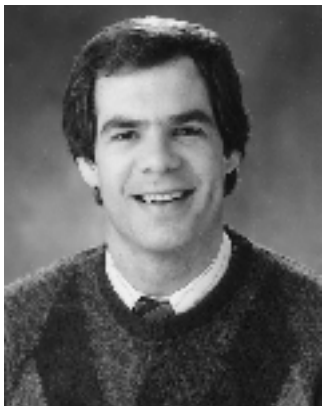
Zhang, X. and O.A. Basaran, "Surfactant Effects on the Nonlinear Deformation and Breakup of Liquid Bridges," AIChE Annual Meeting, Miami Beach, CA, November 12-17, 1995.

Zhang, X. and O.A. Basaran, "Nonlinear Deformation and Breakup of Liquid Bridges in an Electric Field," APS-DFD Meeting, Irvine, CA, November 19-21, 1995.

James M. Caruthers

1977

Professor



Degrees

SB (Chem), Massachusetts Institute of Technology, 1975

SM, Chemical Engineering, Massachusetts Institute of Technology, 1975

PhD, Chemical Engineering, Massachusetts Institute of Technology, 1977

Interests

Viscoelasticity of Solids

Polymer Rheology

Structure-Property Relationships in Polymers

Composites

Awards and Major Appointments

Curtis McGraw, American Society of Engineering Education, 1990

National Research Council: Standing Committee on the Program and Technical Review of the U.S. Army Chemcial 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

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

R. Ramakrishnan, J.F. Pekny and J.M. Caruthers, "A Combinatorial Algorithm for Effective Generation of Long Maximally Compact Lattice Chains," *J. Chemical Physics*, *103,* 7592 (1995).

R. Sy-Siong-Kiao, J.M. Caruthers and K.C. Chao, "Polymer Chain-of-Rotators Equation of State,"*Industrial Engineering Chemistry Research*, *35,* 1446 (1996).

C.R. Novenario, J.M. Caruthers and K.C. Chao, "A Mixing Rule to Incorporate Solution Model into Equation of State," *Industrial & Engineering Chemistry, 35,* 269 (1996).

S.R. Lustig, R.M. Shay, Jr. and J.M. Caruthers, "Thermodynamic Constitutive Equations for Materials with Memory on a Material Time Scale," *Journal of Rheology, 40* (1996).

D.H.S. Ramkumar, J.M. Caruthers, H. Mavridis, and R. Shroff, "Computation of the Linear Viscoelastic Relaxation Spectrum from Experimental Data," *Journal of Applied Polymer Science*, in press.

Invited Lectures

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

"Models for the Prediction of VLE Behavior and Other Thermophysical Properties for Engineering Materials," Herrick Laboratories, Purdue University, August 1995.

"Nonlinear Viscoelasticity in Amorphous Polymers," National Institute of Standards and Technology, Gaithersburg, MD, July 1995.

"Thermoviscoelastic Models for Amorphous Polymers - A Review," Materials Research Society, Boston, MA, December 1995.

"Models for Ninlinear Viscoelasticity: Application of the Adams-Gibbs Configurational Entropy Model," American Physical Society Spring Meeting, St. Louis, MO, March 1996.

"A Model for Nonlinear Viscoelasticity in Amourphous Polymers," Sandia National Laboratories, Albuquerque, NM, July 1996.

Meeting Presentations

"Nonlinear Fluctuations Hydrodynamics of a Viscoelastic Fluid," A.B. Starry and J.M. Caruthers, Society of Rheology, Sacramento, CA, October 1995.

"Nonlinear Viscoelastic Relaxations in the Glass Transition Region," D.S. McWilliams, J. Wang, D.M. Colucci, D.I. Song, and J.M. Caruthers, AIChE Annual Meeting, Miami, FL, November 1995.

"The Effect of Density Fluctuations on Viscoelastic Relaxation in the Glass Transition Region," A.B. Starry and J.M. Caruthers, AIChE Annual Meeting, Miami, FL, November 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

Awards and Major Appointments

Secretary and Director, Board of Directors, American Zhu Kezhen Education Foundation

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

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

Jin, Z., R.A. Greenkorn, and K.C. Chao, "Correlation of Vapor-Liquid Equilibrium Ratio of Hydrogen," *AIChE J., 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 J.*, 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.

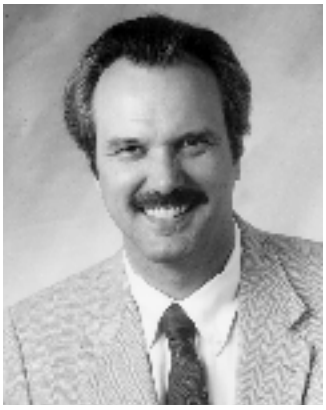
Bereolos, P., J. Talbot, and K.C. Chao, "Simulation of Free Energy without Particle Insertion in the NPT Ensemble," *Molecular Physics*, submitted.

Bereolos, P., K.C. Chao, and J. Talbot, "Molecular Simulation of Fluid Phase Equilibria of Mixtures," *AIChE Journal*, submitted.

W. Nicholas Delgass

1974

Professor and Associate Head of the School



Degrees

BSE, Chemical Engineering, University of Michigan, 1964

BSE, Mathematics, University of Michigan, 1964

MS, Stanford University, 1966

PhD, Stanford University, 1969

Interests

Heterogeneous Catalysis

Selective Hydrogenation over Raney nickel

Partial Oxidation - 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 ^{o}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 Science and 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

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

Chaired Conferences/ Symposia

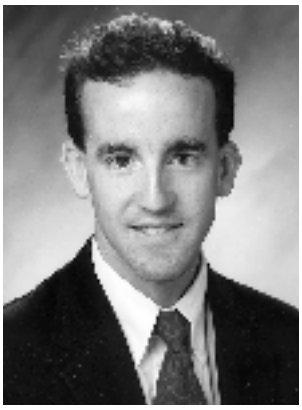
Organizing and Executive Committee, 11th International Congress on Catalysis, Baltimore, MD, June 1996.

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

Francis J. Doyle, III

1992

Assistant Professor



Degrees

BSE, Princeton University, 1985

GPGS, Cambridge University, 1986

PhD, California Institute of Technology, 1991

Interests

Nonlinear Process Identification and Control

Low Order Process Modeling and Nonlinearity Characterization

Biosystems Control

Large Scale Model Predictive Control

Awards and Major Appointments

National Science Foundation National Young Investigator Award, 1992-1997

Office of Naval Research Young Investigator Award, 1996-1999

ASEE Section Outstanding Teacher Award (Illinois/Indiana), 1996

Tau Beta Pi Dean Marion B. Scott Exemplary Character Award, 1996

Research Areas

Nonlinear Process Identification and Control: Linear controller design techniques are widely employed in the chemical/petrochemical industries. In particular, conventional model predictive control (MPC) has enjoyed widespread acceptance and success as an effective technique for dealing with difficult control problems of industrial importance. The appeal of linear MPC is the straightforward handling of process constraints as well as the simplicity arising from the linear models used to approximate process behavior. However, this latter point also constitutes a potential deficiency, because such simple linear models are often inadequate if a more realistic approximation of the usually complex nonlinear processes is desired. On the other hand, the nonlinear control schemes which employ more realistic - and often more complex - nonlinear process descriptions typically sacrifice the simplicity associated with linear techniques in order to achieve improved performance. More importantly, these nonlinear techniques require nonlinear differential equation process models. This limits industrial application since such *first principles* models are not readily available in industrial practice because of a chronic lack of detailed and extensive process knowledge required for their development. In our work, we have considered two approaches to the problem: (i) the selection of appropriate nonlinear models which yield both accurate process representation, as well as tractable nonlinear control-

ler analysis and synthesis, and (ii) the development of a nonlinear anti-windup scheme which relies on linear methods for constraint handling. The philosophy of both approaches is similar - extrapolate the current linear practices in a computationally straightforward way to address the nonlinear problem.

In the first approach, we have developed a direct synthesis scheme for nonlinear model-based control which employs a Volterra model: a nonlinear process representation obtainable from input/output data and similar in form to the conventional MPC model. Furthermore, the scheme gives rise to a controller which clearly decomposes into a conventional linear model-based controller plus a sequence of *analytical* nonlinear "perturbation" or correction terms. In particular, when the process representation is a *second order* Volterra model, the control structure is decomposed into two elements: (i) an optimal linear controller; and (ii) a loop with a second order Volterra term to account for the process nonlinearity. The first step involves the typical *linear* model inversion which characterizes conventional model-based control. The notion of "inversion" that is used here is fairly general and can be relaxed to incorporate penalties on manipulated variables and receding horizon performance criteria. The control engineer is at liberty to select the linear strategy for implementing this step; the correction obtained in the second step involves only the second order Volterra plant model. Thus, only the *linear* inversion involved in obtaining the linear controller is required to synthesize the compensator for the full second order Volterra model. For higher order Volterra models, the successively higher order correction terms (third, fourth, etc.) required in addition to the linear controller are implemented in a similarly straightforward manner. Model identification is facilitated through the use of a compression algorithm coupled with a plant-friendly input sequence to yield a "practical'' approach to the nonlinear model identification problem. The approach uses tailored input sequences which have η distinct levels (thus generalizing the already popular PRBS signals). A second order Volterra model requires 3 levels; 3rd order, 4 levels, etc. This input sequence is coupled with an orthonormal expansion solution for the Volterra kernels (using a Laguerre basis function). The results, which have been applied to a nonlinear polymerizer model, indicated a significant reduction in the amount of data required (translating to less down time for a chemical plant), while yielding vastly improved model accuracy over standard approaches to nonlinear identification.

The second approach is the development of a direct synthesis nonlinear control scheme for constrained uncertain nonlinear process systems. Within the internal model control framework, the resultant controller is composed of the following: (i) a system inverse, and (ii) a filter which facilitates reliability and introduces closed-loop robustness. Results to date include synthesis procedures and analysis results for both SISO and MIMO certain systems. The latest developments in this work are the inclusion of input rate limitations, as well as preliminary results on IMC filter tuning for robustness. This can be contrasted with MPC approaches to the problem which involve programming formulations for a solution. The present approach is a direct synthesis method which can be readily implemented in an advanced distributed control system (DCS) in an industrial setting.

These nonlinear model-based approaches have been applied in simulation to a number of industrial case studies including a fluidized bed reactor, a free radical polymerization reactor, a Kamyr continuous digester, and a high purity binary distillation column.

Low Order Process Modeling and Nonlinearity Characterization: One of the key issues that arises in nonlinear control design is the development of suitable model approximations that are accurate, computationally tractable, and (ideally) physically based. A related issue is the question of whether one need apply nonlinear control methods at all.

We have taken two approaches to the former problem: (i) wave propagation models, and (ii) Hankel reduced models. The wave propagation models are derived from the assumption that certain classes of distributed parameter systems exhibit spatial profiles which maintain thermodynamic stability, and propagate with a shock velocity when perturbed. Typical examples of such processes include distillation columns and packed bed reactors. In our work, we have taken such models, which are typically of very low (approximately 2-4) state dimension, and employed a Kalman filter to estimate the shape parameters. The resulting low order models can be employed in differential geometric synthesis schemes, and applications to a high purity distillation column have indicated that significant performance improvement is possible over linear model-based control schemes. The second model reduction scheme of interest in our work is Hankel model reduction. This scheme has the attraction that a systematic procedure is available for truncating states; however, the remaining states have lost their original physical meaning. We have extended these ideas to nonlinear systems, showing that for systems with a low degree of nonlinearity in the Hankel transformation, one can merely apply the linear Hankel transformation to the original nonlinear problem and achieve excellent results. These ideas have been demonstrated in a state-estimation MPC scheme for a Kamyr continuous digester in which a 1040 state model is reduced to a 40 state model for robust closed-loop performance.

In the general area of modeling and analysis, we have been concerned with the question of the "degree'' of nonlinearity exhibited by a process. The objective of this project is the formulation of a computational tool for process design and process control synthesis which evaluates the *control-relevant* degree of nonlinearity in a given process system. Inherent in this definition is the notion that not all nonlinear systems require nonlinear controllers for stabilization and / or tight performance. For example, there are systems that appear to have highly nonlinear open-loop behavior (*e.g.*, Arrhenius temperature dependence), yet a simple linear controller will yield excellent closed-loop robust performance. The issues of stabilization and closed-loop performance are clearly tied to the intrinsic characteristics of the particular process in question. Indeed, as demonstrated by many researchers, there exist classes of nonlinear plants that are optimally and robustly controlled by a linear controller. Clearly, a simple analysis of the open-loop system does not include all the information needed to determine the control relevant nonlinearity of a system. In particular, *it does not include the effects of a performance objective or the costs of control action.*

Our preliminary results employ an optimal control based method to develop a relevant operator for control-relevant nonlinearity assessment. The operator development draws from Lagrangian optimization principles. We have formulated a nonlinear operator using optimal control theory which captures the degree of nonlinear compensation required. This operator can be evaluated with any standard tool for *open-loop* process nonlinearity measurement; in our work we employ the coherence suppression as a measure of system nonlinearity. The coherence analysis yields a frequency dependent scalar which ranges from 0.0 (complete linear suppression - i.e., very nonlinear) to 1.0 (no suppression - i.e., completely linear). Our preliminary results have focused on mathematical systems (Wiener and Hammerstein systems) as well as simple batch reaction systems. In the case of the batch reaction system, the *control-relevant* nonlinearity was characterized as a function of several key engineering variables: (i) performance weight on setpoint tracking, (ii) magnitude bounds on manipulated variable, and (iii) frequency content of the input (driving) signal.

Biosystems Control: In the broad area of biosystems control, we are concerned with two directions of technology transfer: (i) how can engineers learn from biological architectures, and (ii) how can engineers contribute to medical therapies. The quest for global competitiveness has driven chemical companies in the U.S. to produce higher quality products at lower prices, while maintaining ever tightening environmental emissions constraints. An effective means to achieving these goals is advanced control strategies. The present industrial approaches for automated process operations, however, fall considerably short of achieving such demanding performance objectives. One source of inspiration for new strategies is biological control systems. It has been recognized for centuries that the human body is effectively a complex chemical factory, composed of many highly interactive multivariable subsystems. It has also been demonstrated that natural "controllers'' achieve tight regulation of these systems under a variety of conditions in order to meet stringent performance requirements - thus achieving r*obust performance*. Hence, there is a clear incentive to pursue a *neuromimetic* approach to control design - to reverse engineer one of these natural control loops to introduce new paradigms for process control. In the words of A.G.J. MacFarlane - "*major advances are taking place in neurophysiology which will surely provide pointers to possible ways of developing high functionality controllers.*'' In this research project, we have chosen a simple biological control architecture, the *baroreceptor vagal reflex*. This system, which is responsible for the short term regulation of blood pressure, displays a rich range of nonlinear dynamic behavior. At the sensory limb, neurons receive synaptic input as the blood vessels are stretched and this information is projected onto second order neurons in the nucleus tractus solitarii (NTS). This information is then processed in the nucleus ambiguus where neuronal output drives the motor limb: cardiac rate and stroke volume. Thus, as blood pressure increases above a target level, a signal is generated by a neural controller which lowers the heart rate. We have had initial success in two particular areas: (i) abstraction of computational principles in baroreflex neurons for applications in nonlinear model-based control, and (ii) design of a novel control-scheduling algorithm based upon the second order structure in the baroreflex. The latter project has focused on the "dynamic scheduling'' exhibited by the

baroreceptor neurons in translating blood pressure to the NTS neurons in the brain. The behavior has been emulated in the form of a grade transition control policy for a complex polymerization reactor, and has yielded substantially improved performance over the traditional gain scheduling strategy typically employed in industry. Furthermore, recent experimental evidence from our group has indicated the presence of a previously unknown control loop in the baroreflex which is localized in the heart and does not involve a relay through the brain. This *axon reflex* is important for two reasons: (i) it points to opportunities in process engineering for intelligent sensors and intelligent control valves, and (ii) it points to the rich hierarchical nature of the processing which underlies blood pressure control. In order of decreasing scale, these processes include supervisory levels (hormonal and endocrine system), advanced control levels (parasympathetic and sympathetic systems), local control (axon reflex), and autoregulatory systems (second messenger species in neuron cells). Engineering problems share similar hierarchical structures, with high level discrete decision variables that are driven by low level continuously measured variables. *A principal aim of our work is to abstract the integration principles which unite these processing layers in biological systems to improve computer integrated process operations.*

The second theme in the biosystems research is the application of control engineering principles to medical therapy - specifically the management of diabetes; this represents an active collaboration with Professor Nicholas Peppas. In this work, novel self-regulated devices for insulin delivery to diabetic patients are proposed. These controlled release devices are based upon glucose- and pH- sensitive hydrogels which release insulin at desirable levels. The strategy consists of three distinct components: (i) the development of models that represent healthy and diabetic patients, models for the natural biocontrol loop, and a model for the polymeric device; (ii) the employment of a detailed process model in a model-based control strategy (model predictive control) to evaluate the maximum achievable performance of conventional drug delivery technologies (*i.e.*, implantable pumps); and (iii) the synthesis of glucose-sensitive polymers by immobilizing glucose oxidase in pH-sensitive graft copolymers of poly(methacrylic acid-g-ethylene glycol), henceforth designated as P(MAA-g-EG). The three components are closely linked as the modeling studies will provide a basis for mathematical analysis of the open-loop control problem (diabetic patient), a reference for achievable control (healthy patient) and a template for a controller (biocontroller) which, in turn, will be used to guide the optimal design of the polymeric device. The results of this work will contribute to the medical field by providing new therapies or improved methods of insulin delivery in diabetic patients. These new therapies will facilitate the accurate and timely delivery of insulin as needed by the patient, avoiding both premature and excessive delivery. The implications of such improved control are the eradication of the short term symptoms of poor insulin delivery in diabetic patients, including: (i) hyperglycemia with the associated symptoms of weight-loss and fatigue, and (ii) hypoglycaemia which may lead to loss in concentration or even coma. In addition, the longer term effects of nephropathy and retinopathy may be alleviated.

Large Scale Model Predictive Control: (This project is a joint effort with Professor Joseph Pekny). Linear model predictive control has

been successfully applied in the chemical and petrochemical industries for over a decade in the context of single unit control. The appeal of this approach can be attributed to the flexible handling of constraints on process variables and the relative ease of tuning for increased robustness. In the decade since linear model predictive control was first introduced, there has been a dramatic improvement in computational power coupled directly with more efficient algorithms for mathematical programming. In particular, there have been several examples demonstrating the power of optimization algorithms tailored to exploit problem structure. The object of the proposed research is to develop tailored algorithms for the solution of optimization problems arising in large linear model predictive control applications, for example, integrated management of several process units and/or control of complex units such as paper machines. An important part of the algorithm customization will be the distributed solution of the resulting mathematical programming problems using a collection of workstations that is analogous to the type of distributed computing power available for the control of chemical plants. A key promise of the proposed approach is the ability to integrate economic process management considerations directly into control schemes. This will result directly from being able to solve the large control problems that result when the plant is viewed in its entirety. From an intellectual viewpoint, the proposed research provides a means of integrating work at the relatively long time scales of process scheduling and planning with the relatively short time scales of process control. Industrial evidence suggests that taking a consistent view of both levels will result in substantial economic benefits by removing mismatches in the separate treatment of related problems. Thus the work will result in a significant increase in the scope of model predictive control applications and a new class of mathematical programming algorithms tailored for an important family of problems within the chemical industry.

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Bassett, M.H., P. Dave, F.J. Doyle III, G.K. Kudva, J.F. Pekny, G. V. Reklaitis, S. Subrahmanyam, D.L. Miller and M.G. Zentner, "Perspectives on Model Based Integration of Process Operations," *Comp. Chem. Eng.*, 20, 821-844, 1996.

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Kwatra, H., F.J. Doyle III, J.S. Schwaber and I. Rybak, "A Neuromimetic Dynamic Scheduling Algorithm for Control: Analysis and Applications," *Neural Computation*, in press, 1996.

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Doyle, F.J. III, T.A. Kendi and V. Venkatasubramanian, "PCM: A MATLAB-Based Set of Modules for Undergraduate Process Control," *Comp. Appl. Eng. Ed.*, in press, 1996.

Doyle, F.J. III, M.A. Henson, B.A. Ogunnaike, J.S. Schwaber and I. Rybak, "Neuronal Modeling of the Baroreceptor Reflex with Application in Process Modeling and Control," in Neural Networks for Control, D.L. Elliott, Editor, Ablex Publishing, in press, 1996.

Doyle, F.J. III and M.A. Henson, "Nonlinear Systems Theory," in Nonlinear Process Control, M.A. Henson and D.E. Seborg (eds), McGraw-Hill, in press, 1996.

Invited Lectures

"Nonlinear Process Control: Which Way to the Promised Land?" Chemical Process Control V, Lake Tahoe, CA, 1996.

"Reverse Engineering a Biological Reflex for Applications in Process Control," University of Cincinnati, Cincinnati, OH, February 1996.

"Neuromorphic Engineering: Unraveling a Biological Reflex for Applications in Process Control," Queen's University, Kingston, Canada, April 1996.

"Plant Design for Operability: An Introduction to the Available Mathematical Tools," AIChE/ISA Technochem '96, Houston, TX, May 1996.

Chaired Conferences/ Symposia

Session Chairman "Robust Control of Linear Systems," *European Control Conference*, Rome, Italy, September 1995.

Session Co-chairman "Applied Neurobiology," *AIChE Annual Meeting*, Miami, CA, November 1995.

Session Chairman "New Directons for Academic Research," *CPC V Meeting*, Lake Tahoe, CA, January 1996.

Programming Committee, *Chemical Process Control V Meeting*, Lake Tahoe, CA, January 1996.

Meeting Presentations

Kendi, T.A. and F.J. Doyle III, "An Anti-windup Scheme for Input Output Linearization," *Proc. European Control Conference*, Rome, Italy, September 1995.

Peppas, N.A., F.J. Doyle III and C.M. Dorski, "Recent Developments in Insulin Delivery and Control Using Hydrogel Systems," presented at *First Spanish-Portuguese Conf. on Controlled Drug Delivery*, Santiago de Compostella, Spain, 1995.

Cheng, Z., T.L. Powley, J.S. Schwaber and F.J. Doyle III, "Vagal Afferent Innervation of the Rat Heart Reconstructed with Laser Confocal Microscopy: Local Reflex Circuits?" presented at N*euroscience Annual Meeting*, San Diego, CA, 1995.

Shaw, A.M. and F.J. Doyle III, "Nonlinear Control Design Using a Dynamic Neuron Empirical Model," presented at *AIChE Annual Meeting*, Miami, FL, 1995.

Dave, P., F.J. Doyle III and J.F. Pekny, "Specialized Mathematical Programming Methods for Model Predictive Control of Large Scale Systems," presented at *AIChE Annual Meeting*, Miami, FL, 1995.

Aoyama, A., F.J. Doyle III and V. Venkatasubramanian, "Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control," presented at *AIChE Annual Meeting*, Miami, FL, 1995.

Kwatra, H.S. and F.J. Doyle III, "Dynamic Gain Scheduled Control," presented at *AIChE Annual Meeting*, Miami, FL, 1995.

Doyle III, F.J., T.A. Kendi and V. Venkatasubramanian, Purdue Control Modules (PCM): A MATLAB-Based Package for Undergraduate Process Control," presented at *AIChE Annual Meeting*, Miami, FL, 1995.

N.A. Peppas, F.J. Doyle, C.M. Dorski and K. Podual, "Intelligent Hydrogel Systems for Protein and Drug Release with Feedback Control," *Proc. 3rd US-Japan Symp. on Drug Delivery Systems*, Maui, December 1995.

Doyle III, F.J. and F. Allgöwer, "Nonlinear Process Control: Which Way to the Promised Land?" P*roc. CPC V*, Lake Tahoe, CA, January 1996.

Dorski, C.M., F.J. Doyle III and N.A. Peppas, "Glucose-Responsive Complexation Hydrogels," *Polymer Prepr., 37 ACS Meeting*, New Orleans, LA, March 1996, p. 475-476.

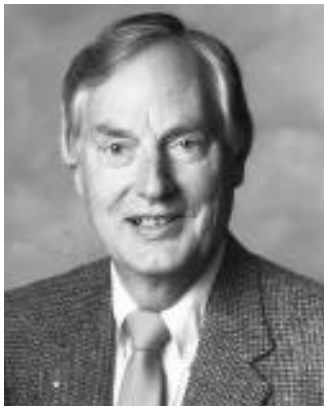
Doyle III, F.J., P.A. Wisnewski and C. Primus, "Measurement Selection Issues for the Model Predictive Control of a Kamyr Digester," *Proc. Control'96*, Halifax, April 1996.

Wisnewski, P.A. and F.J. Doyle III, "A Reduced Model Approach to Estimation of Kappa # for Control of a Kamyr Digester," *ESCAPE,* Rhodes, Greece, May 1996.

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.

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R.E. Eckert, "Applied Statistics: Are Chemical Engineering Educators Meeting the Challenge? A Survey of Statistics in the Chemical Engineering Curricula," *Chem. Eng. Education*, **30**, No. 2, 122-125, 1996.

Albright, L.F., M.K. Sood, and R.E. Eckert, "Modeling Nitronium Ion Concentrations in Nitric Acid-Sulfuric Acid-Water Mixtures," in *Nitration: Recent Laboratory and Industrual Developments*. Edited by Lyle F. Albright, Richard V.C. Carr and Roger J. Schmitt, ACS Symposium Series 623, 201-213, Washington, DC, 1996.

Elias I. Franses

1979

Professor

Degrees

DEng. National Technical University, Athens, 1974

PhD, University of Minnesota, 1979

Interests

Adsorption and Tension Equilibria and Dynamics of Surfactants, Lipids, and Proteins

Applications to Lung Surfactant Formulations, Foaming, and Cleaning Processes

Transport and Ion Exchange in Thin Organic Films; Barrier and Membrane Materials

Infrared Spectroscopy and Ellipsometry of Thin Films at Solid and Fluid Interfaces

Awards and Major Appointments

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

International Advisory Committee, International Symposium on Micelles, Microemulsions, and Monolayers: Quarter Century Progress and New Horizons, Gainesville, FL, August 1995

Research Areas

Equilibrium Adsorption and Tension of Aqueous Surfactant or Ionic Mixtures: Binary and multicomponent adsorption at air / water, oil / water, gas / solid, and liquid / solid interfaces is important in foams, emulsions, detergency and cleaning processes, coating flows, catalysis, and certain separation methods. Many practical surfactant or other systems involve molecules of different size, shape, adsorption capacity, adsorption strength, and ionic character (anionic, nonionic, etc). We have developed guidelines for determining thermodynamically consistent adsorption isotherms for mixtures. Then, using data on adsorption or tension on single adsorbates, we develop rigorous thermodynamic models accounting for mixing in monolayers, and for relative size and nonideal intermolecular interactions in the monolayer. Important new results are: (i) new surface isotherms for mixtures; (ii) conditions for tension synergism (mixture better than components) in tension below and above the cmc; (iii) conditions for adsorption synergism. The project is continuing with direct probing of monolayers with spectroellipsometry and external reflection infrared spectroscopy. The results are applied to formulating effective cleaning

products, to controlling foaming, and to lung surfactants. Moreover, analogous nonideal-adsorbed solution models are being developed for ions bound to surfaces or surface monolayers (with F.A. Siddiqui and Prof. N.-H.L. Wang).

Dynamic Adsorption and Tension of Aqueous Surfactants, Lipids, and Proteins: Many fast processes such as foaming, coating flows, cleaning, and breathing (lung surfactants - a biomedical engineering project) are affected more by adsorption / tension dynamics than by adsorption / tension equilibria. In one project (with Dr. C.H. Chang), we have studied and reviewed the past and current literature on dynamics of adsorption, models, data, and mechanisms. We also reviewed (with Prof. O.A. Basaran and Dr. C.H. Chang) the most effective techniques for measuring dynamic surface tension, over time scales of 10^{-3} - 10^{5} s. The dynamics depends on the thermodynamics of adsorption and mass transfer properties: convection, diffusion, adsorption, and desorption, at constant or varying surface area. New models are being developed to account for mixture effects and extremely low tensions (< 10 mN / m) produced under nonequilibrium conditions (with Dr. C.H. Chang). The models are tested against surface tension data, ellipsometry data, and data using radiotracers (for a protein, BSA, and its derivatives). The effect of surface hydrophobicity on adsorption at the air / water surface was studied systematically for the first time (with Prof. G. Narsimhan and D. Cho). Dynamic adsorption / tension models for surfactants of different size are being developed (with F.A. Siddiqui). The effect of surfactant chain length on tension is being studied for three important classes of surfactants and lipids: lecithin phospholipids, alcohols, and salts of fatty acids (with S.Y. Park, K. Coltharp, S. Myrick, X. Wen, and A. Pinazo). We elucidated the roles of dispersed particles (crystallites, liposomes, vesicles) on the tension dynamics. We discovered two systems which can produce low tensions (possibly relevant to lung surfactants), while being molecular solutions or dispersions of liposomes. Finally, we established the existence of the low nonequilibrium tensions and explained them via simple transport / thermodynamic models. Our current efforts emphasize: developing applications in cleaning and foaming; (ii) better understanding of interactions in mixtures; and (iii) more direct probing of the surface using optical and spectroscopic tools; and (ii) more detailed or refined control of dynamic surface tension, with goals of formulating more effective and less costly lung surfactant replacement drugs.

Production and Characterization of Ultrathin Organic Films: Such films are important in microlithography, nonlinear optical materials, barrier materials, and membrane materials. In one project, we evaluate the effect of processing method æ regular casting, spin casting, or Langmuir-Blodgett (LB) deposition æ on the thickness range, film quality, and film permeability. We have found out the state of water (monomer units, hydrogen-bonded clusters, etc.) in polymer (PMMA) membranes and followed the transport dynamics in situ by infrared spectroscopy (with D.J. Ahn and P. Sutandar). The film surface roughness, optical properties, and density are examined with profilometry and ellipsometry and are related to their transport properties (with C.B. Walsh). The project now is headed toward studies of permeability and selectivity for polymer films (PMMA) or LB films of fatty acids and their salts. New models are being developed to interpret ellipsometry experiments, not only for the average film properties but

for voids and surface roughness. Ellipsometry is also being applied to characterize adsorption (both equilibrium and dynamic) at air/water interfaces. Moreover, in situ FTIR is used for probing film microstructure during transport. Both techniques are used to probe swelling dynamics and develop transport models for solute permeation.

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Sutandar, P., D.J. Ahn and E.I. Franses, "Microstructure and Water Transport in Spin-Cast Films of Poly(hexylmethacrylate Azobenzene Sulfone), *Thin Solid Films, 263*, 134-144, 1995.

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Puig, J.E., J.F.A. Soltero, E.I. Franses, L.A. Torres and P.C. Schulz, "The State of Water and Surfactant in Surfactant-Based Lyotropic Liquid Crystals," in *Surfactants in Solution*, Mittal, K.L. and Chattopadhyay (eds), Plenum Press, N.Y., in press, 1996, invited paper.

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Siddiqui, F. and E.I. Franses, "Surface Tension and Adsorption Synergism for Solutions of Binary Surfactants," *Ind. Eng. Chem. Res.*, in press, 1996.

Bernardin, J.D., I. Mudawar, C.B. Walsh and E.I. Franses, "Contact Angle Temperature Dependence for Water Droplets on Practical Aluminum Surfaces," *Intern. J. Heat Mass Transfer*, accepted, 1996.

Invited Lectures

"Dynamic Properties of Spread and Adsorbed Monolayers at the Air/Water Interface," (invited talk, with D.J. Ahn, C.-H. Chang, J.B. Chung, K.A. Coltharp, and S.Y. Park), International Symposium on Micelles, Microemulsions, and Monolayers: Quarter Century Progress and New Horizons, Gainesville, FL, August 1995.

"Equilibrium and Dynamic Adsorption of Surfactants at the Air/Water Interface," Johnson and Sons Company, Racine, WI, October 1995.

"Equilibrium and Dynamic Adsorption and Tension of Binary Surfactants at the Air/Water Interface," (with F.A. Siddiqui; presented by F.A. Siddiqui), American Chemical Society 1996 Central Regional Meeting, Dayton, OH, June 1996.

"Dynamic Tension Behavior of Aqueous Alcohol Dispersions," (with S.H. Myrick and S.Y. Park; presented by S.H. Myrick), American Chemical Society 1996 Central Regional Meeting, Dayton, OH, June 1996.

Meeting Presentations

"Adsorption and Tension of Aqueous Surfactant Mixtures," (poster paper, with F.A. Siddiqui; presented by F.A. Siddiqui), International Symposium on Micelles, Microemulsions, and Monolayers: Quarter Century Progress and New Horizons, Gainesville, FL, August 1995.

"Adsorption Dynamics of Native and Alkylated Derivatives of Bovine Serum Albumin at Air/Water Interfaces," (with D. Cho and G. Narsimhan; presented by D. Cho), AIChE Annual Meeting, Miami Beach, FL, November 1995.

"Adsorption Equilibria and Surface Tension of Aqueous Surfactant Mixtures," (with F.A. Siddiqui), AIChE Annual Meeting, Miami Beach, FL, November 1995.

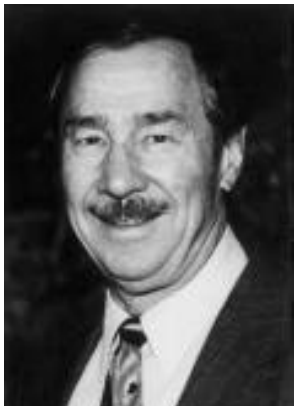
"Nonideal Adsorbed Solution Model: Predictions of Concentration Ranges for Adsorption and Tension synergism Below and Above the CMC," (with F.A. Siddiqui), 11th International Symposium on Surfactants in Solution. Synergism and Mixtures, Jerusalem, Israel, June 1996.

Robert A. Greenkorn

1965

R. Games Slayter Distinguished Professor of Chemical Engineering

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



Degrees

BS, University of Wisconsin, 1954

MS, University of Wisconsin, 1955

PhD, University of Wisconsin, 1957

Interests

Flow Phenomena in Porous Media

Pollution Prevention

System Modeling

Awards and Major Appointments

Editorial Board 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

Director, Purdue Technical Assistance Program

Research Areas

Magnetic Resonance Imaging of Mixing During Flow in Heterogeneous Porous Media: The displacement of pollutants in soils and underground reservoirs is a promising method for environmental restoration.

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

Pollution Prevention - A Limited Automatic Information Retrieval System: Literature searches of databases are usually accomplished with a human intermediary familiar with database search methods. The user of the information provides the intermediary with key words or phrases for use in a search. A search may use the Boolean operators, “and, “ “or” and “not” to limit the recall of stored material - the proportion of relevant material. The more limited the recall the less precision, the proportion of retrieved material that is relevant. The goal of this research is to determine strategies for automating information retrieval. The specific objectives are to: (1) Design an automatic updating strategy for previous pollution prevention searches in five specific areas, (2) Program this strategy, (3) Test the results with the existing information search and assessment, (4) Use the system to provide technology updates for the five areas on the WWW.

System Modelling - A Model of University Enrollment, Research, Classes and Costs: Currently four linear models have been constructed for enrollment, research, classes and costs at Purdue University. These are being combined into a model system. Each department of the university is modeled. The models will be enlarged to include classes at six levels (freshman, sophmore, junior, senior, dual level and graduate classes) and by lecture, recitation, and laboratory.

Publications

Sternberg, S.P.K., J.H. Cushman and R.A. Greenkorn, “Laboratory Observation of Non-Local Dispersion,” Trans. P.M., 1996, in press.

Sternberg, S.P.K., J.H. Cushman and R.A. Greenkorn, “Random Walks in Prefractal Porous Media,” *AIChE.J*, 42 #4, 921-926, 1996.

Jin, Z., R.A. Greenkorn and K.C. Chao, “Correlation of Vapor-Liquid Equilibrium Ratio of Hydrogen,” *AIChE.J*, 41 #6, 1602-1604, 1995.

Meeting Presentations

Roth, C.B. and R.A. Greenkorn, “Review, Assessment and Transfer of Pollution Prevention Technology in Plastics and RFC Industries,” Proc. Ind. Waste Conf., Purdue University, West Lafayette, IN, May 1996.

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: Serum bilirubin determination by skin reflectance: (with Professor David DeWitt, Mechanical Engineering). This work is now being done by SpectRx in Norcross, Georgia. They are evaluating our previous work with the goal of working in collaboration with us or using us as consultants.

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

"Moisture Transport in Shrinking Gels During Saturate 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.

Hilary S. Lackritz

1991

Associate Professor

Degrees

BS, Northwestern University, 1985

PhD, Materials Science & Engineering, Northwestern University, 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 Chemical Society / Optical Society of America (ACS / OSA) Symposium on Organic Thin Films for Photonic Applications: International Advisory Committee, (1994-)

ACS Program Chair- 1995 Portland OSA meeting

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

Research Areas

Polymer physics of electro-optic polymers for photonic devices: New classes of polymeric nonlinear optical (NLO) materials are being developed that utilize 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 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 utilized 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.

Nonlinear optical studies probing diffusion at polymer interfaces: Novel nonlinear optical methods will be developed to examine continuously polymer / polymer diffusion at interfaces in real time with highly surface sensitive techniques as a function of polymer physical, chemical, and processing modifications. Interfaces are an important area of study in many areas of polymer engineering, and particularly in the materials engineering of organic optical and electronic materials.

In order to develop advanced polymeric materials for integrated optical applications including optical sensors and multilayer waveguides it is important to understand diffusion and interactions at polymer/polymer interfaces. Optical techniques can be used to study continuously the diffusion across interfaces in multilayer polymer systems in a non-invasive, non-destructive method that is sensitive to small changes in bulk or local properties. Recent studies have shown that nonlinear optical methods can be used to study mobility and polymer physics phenomena at the local level.

The primary nonlinear optical technique that will be utilized in these experiments is surface second harmonic generation (SSHG). Second harmonic generation, the conversion of light frequency w to light of frequency 2w, occurs only at noncentrosymmetric sites, such as the interface between two polymers or any interface between materials with different indices of refraction. SHG is thus highly surface sensitive. Because it is a coherent optical process, SSHG is highly directional. In situ tests can continuously monitor changes in the optical properties at the interface without disturbing the sample, which can be modified by temperature and other external variables during experimentation. This technique, which can be used remotely to study all interfaces accessible by light, has high temporal, spectral, and spatial resolution and can be performed with the sample in a variety of environments. Thus, a combination of linear and nonlinear optical techniques will provide an excellent, novel method for examining the diffusion across polymer/polymer interfaces.

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, I will develop surface second harmonic generation to characterize the dynamics at the metal/polymer interface. With 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

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

Pasmore, T., J. Talbot and H.S. Lackritz, "Monte-Carlo Simulations of Electric Field Hopping in Doped Polymer Thin Films," Mol. Cryst. Liq. Cryst. Sci. Tech. B: Nonlinear Optics, 10, 295, 1995.

Zhuang, X., H.S. Lackritz and Y.R. Shen, "Photo-isomerization of Polymer Monolayers and Multilayers on Water," Chem. Phys. Lett., 246, 279-284, 1995.

Sullivan, L.A. and H.S. Lackritz, "Dynamic Mechanical Analysis and Dielectric Relaxation for Second Order Nonlinear Optical Applications," Materials Research Society Symposium Series, 392, 69-75, 1995.

Chen, F., S. Subramanyan and H.S. Lackritz, "Photopolymerization Dynamics of Acrolein onto Metal Substrates Using Surface Second Harmonic Generation," Materials Research Society Symposium Series, 1995, 385, 3-9.

Pasmore, T.A., J. Talbot and H.S. Lackritz, "Charge Transport through Polymer Thin Films for Second Order Nonlinear Optics," IEEE Conference on Electrical Insulation and Dielectric Phenomena Annual Report (Proceedings), 95CH35842, 646-649, 1995.

Fu, C.Y.S., H.S. Lackritz, D.B. Priddy, Jr. and J.E. McGrath, "Polymer Physics and Structure / Property Relationships of Thermally Stable Polyarylene Ethers for Second Order Nonlinear Optics," Chem. Mater., 8, 514-524, 1996.

Fu, C.S.Y., M.H. Ostrowski and *H.S. Lackritz, "Dielectric Relaxation Studies of Polymeric Nonlinear Optical Materials" in Dielectric Spectroscopy of Polymeric Materials, Runt, J. P. and Fitzgerald, J. J., Eds. ACS Symposium Series, American Chemical Society, Washington, D.C., in press. (Invited Publication)

Fu, C.Y.S., H.S. Lackritz, D.B. Priddy, Jr. and J.E. McGrath, "Effects of Chromophore Functionalization and Physical Aging during Poling on Chromophore Orientational Dynamics in Polyarylene Ethers for Second Order Nonlinear Optics," Macromolecules, in press.

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

Fu, C.Y.S., H.S. Lackritz, D.B. Priddy, Jr. and J.E. McGrath, "Polymer Physics and Structure / Property Relationships of Thermally Stable Polyarylene Ethers for Second Order Nonlinear Optics," Chem. Mater., in press.

Liu, L.Y. and H.S. Lackritz, "The Effects of Electric Field and Polymer Relaxation on the Rotational Brownian Motion of Chromophores in Polymer Films for Second Order Nonlinear Optics," Nonlinear Optics, in press.

Invited Lectures

"Design and Development of Polymers for Second Order Nonlinear Optics," presented at Kyoto Institute of Technology, Kyoto, Japan, July 1995 (Invited Lectureship).

"Polymer Relaxations and Electric Field Effects in Polymers for Second Order Nonlinear Optics," presented at the International Conference on Organic Nonlinear Optics in Gunma, Japan, July 1995.

"Polymer Physics and Electric Field Effects in Poled Polymers for Second Order Nonlinear Optics," presented at the International Conference on Advanced Materials, International Union of Materials Research Societies, Cancun, Mexico, August 1995.

"Second Order Nonlinear Optical Polymer Dynamics," presented at Miami University, Materials Science Program, Cincinnati, OH, September 1995.

"The Characterization of Polymer Dynamics in Poled Second Order Nonlinear Optical Polymers," presented at the Pacific Polymer Conference, Kauai, HI, December 1995.

"The Characterization of Polymer Dynamics in Poled Second Order Nonlinear Optical Polymers," presented at Princeton University, Department of Chemical Engineering, Princeton, NJ, January 1996.

"Polymer Physics and Electric Field Effects in Poled Polymers for Second Order Nonlinear Optics," presented at Notre Dame University, Department of Chemical Engineering, South Bend, IN, January 1996.

"Optical Characterization of Polymer Dynamics," presented at Northwestern University, Department of Chemical Engineering, Evanston, IL, February 1996.

"Electric Field Effects in Electro-optic Polyimides," presented at Wright-Patterson Air Force Base, Dayton, OH, February 1996.

"Electric Field Effects in Polymer Thin Films for Second Order Nonlinear Optical Applications," presented at Antec 96, Society of Plastics Engineers, Indianapolis, IN, May 1996.

Chaired Conferences/ Symposia

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

ACS Program Co-Chair- 1995 Portland OSA meeting.

ACS Program Co-Chair- 1996 Orlando ACS meeting.

Symposium Co-Chair- 1997 Long Beach OSA meeting.

Symposium Co-Chair, Lead- 1998 Miami Beach ACS meeting.

Session Chair - "Conjugated and Conducting Polymers," American Chemical Society Meeting, Chicago, IL, August 1995.

Session Chair - "Polymer Relaxation Dynamics," American Physical Society Meeting, St. Louis, MO, March 1996.

Session Chair - Antec 96, Society of Plastics Engineers, Indianapolis, IN, May 1996.

Editorial Service

American Physical Society (Division of High Polymer Physics APS DHPP)

Publications Committee, (1993-)

Publication Committee Chair, 1998

Guest Editor: Journal of Polymer Science: Polymer Physics 1998 APS DHPP Special Issue

Meeting Presentations

"Electric Field Effects in Poled Polymer Thin Films," presented at the American Chemical Society / Optical Society of America Symposium on Organic Films for Photonic Applications (at OSA national meeting) in Portland, OR, September 1995.

"Electro-optic and Second Harmonic Generation Studies of Dye-Doped Polymers," presented at the American Chemical Society / Optical Society of America Symposium on Organic Films for Photonic Applications (at OSA national meeting) in Portland, OR, September 1995.

"Studies of Photopolymerization at Metal Surfaces," presented at the American Chemical Society / Optical Society of America Symposium on Organic Films for Photonic Applications (at OSA national meeting) in Portland, OR, September 1995.

"Charge Transport through Polymer Thin Films for Second Order Nonlinear Optics," IEEE Conference on Electrical Insulation and Dielectric Phenomena, Virginia Beach, VA, October 1995.

"Thermal Stability Studies of DCM-Polyimide System for Second-Order Nonlinear Optical Applications," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

"Steady State Charge Transport through Molecularly Doped Polymer Thin Films for Second Order Nonlinear Optics," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

"Vapor Phase Photopolymerization of Acrolein on Metallic Substrates," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

"Electric Field Effects in Poled Polymer Thin Film Systems," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

"Theoretical Study of SHG Intensity Decay in Dye-Polymer Systems During Physical Aging," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

"Photo-Isomerization of Polymer Monolayers and Multilayers on Water," presented at the American Physical Society national meeting in St. Louis, MO, March 1996.

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

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

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

Manufacturing Problem Solving Using Uncertain Data: Fundamental physics shows that uncertainty is an integral part of reality. At the macroscopic level this uncertainty manifests itself as an inability to measure quantities with arbitrary precision and unplanned events. In conjunction with complexity, uncertainty is a major impediment to the efficient management of manufacturing resources. An important means for coping with uncertainty is the development of strategies that are effective over a large fraction of possible outcomes. The goal of our research is the formation and investigation of such strategies in the context of their deployment in manufacturing decision support systems. This research encompasses methods for incorporating uncertainty directly into optimization models, the development of systematic "what-if" paradigms, Mixed Integer Linear Programming (MILP) sensitivity analysis, and parametric optimization. A major practical goal of this research is the ability to dynamically answer questions such as: how much inventory or idle capacity should be kept as an insurance policy, when should an order be promised for delivery to a customer, is external (third-party) manufacturing an attractive option, which types of contractual features are desirable with suppliers and customers to best

match process physics, when should existing facilities be cannibalized for new production capacity instead of building facilities, and what will be the impact of implementing a proposed product? A natural outcome of this research is the ability to demarcate and respond to operational difficulties due to uncertainty, process complexity, and the interaction between the two phenomena.

Publications

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*, Vol. 7, No. 3, pp. 298-320, 1995.

Subrahmanyam, S., M.H. Bassett, J.F. Pekny, G.V. Reklaitis, "Issues in Solving Large Scale Planning, Design, and Scheduling Problems in Batch Chemical Plants," Computers and Chemical Engineering, Vol. 19, Supplemental, pp. S577-S582, 1995.

Ramakrishnan, R., J.F. Pekny, and J.M. Caruthers, "A Combinatorial Algorithm for Effective Generation of Long Maximally Compact Lattice Chains," *Journal of Chemical Physics*, Vol. 103, No. 17, pp. 7592-7605, 1995.

Bassett, M.H., P. Dave, F.J. Doyle III, G.K. Kudva, J.F. Pekny, G.V. Reklaitis, S. Subrahmanyam, D.L. Miller and M.G. Zentner, "Perspectives on Model Based Integration of Process Operations," *Computers and Chemical Engineering*, Vol. 20, No. 6/7, pp. 821-844, special issue publishing selected refereed papers from the Fifth International Symposium on Process Systems Engineering, 1996.

Subrahmanyam, S., G.K. Kudva, M.H. Bassett, and J.F. Pekny, "Application of Distributed Computing to Batch Plant Design and Scheduling," *AIChEJ*, Vol. 42, No. 6, pp. 1648-1661, 1996.

Ramachandran, B. and J.F. Pekny, "Dynamic Matrix Factorization Methods for Using Formulations Derived From Higher Order Lifting Techniques in the Solution of the Quadratic Assignment Problem," *State of the Art in Global Optimization*, C.A. Floudas and P.M. Floudas (editors), Kluwer Academic Publishers, pp. 75-92 1996.

Subrahmanyam, S., J.F. Pekny, and G.V. Reklaitis, "Decomposition Approaches to Batch Plant Design and Planning," *Industrial and Engineering Chemistry Research*, Vol. 35, pp. 1866-1876, 1996.

Meeting Presentations

R. Wajge, J. Wilson, J. Pekny, and G. Reklaitis "Design of Optimal Feed and Reflux Policy for Multicomponent Reactive Distillation," AIChE Fall National Meeting, Miami Beach, FL, 1995.

R. Ramakrishnan and J. Pekny, "A Generation Scheme for Compact Lattice Chains Which Eliminates the Problem of Attrition," AIChE Fall National Meeting, Miami Beach, FL, 1995.

B. Ramachandran and J. Pekny "Solution of Sequencing Problems With Non-Consecutive State Dependent Changeover Costs and Production Release Times and Deadlines," AIChE Fall National Meeting, Miami Beach, FL, 1995.

W. Gooding and J. Pekny, “NETG: A Network Embedded-Time Graph Formulation for Process Scheduling Problems,” AIChE Fall National Meeting, Miami Beach, FL, 1995.

F. Doyle III, P. Dave, and J. Pekny, “Specialized Mathematical Programming Methods in the Model Predictive Control of Large Scale Systems,” AIChE Fall National Meeting, Miami Beach, FL, 1995.

S. Subrahmanyam, J. Pekny, and G. Reklaitis, “An Integrated Approach to Economic and Environmental Issues in the Design of Batch Chemical Processes,” AIChE Spring National Meeting, New Orleans, LA, 1996.

P. Bunch and J. Pekny, “An Exact Primal Dual Based Algorithm for the Perfect B-Matching Problem,” Federation of Operational Research Societies (IFORS) 14th Triennial Conference, Vancouver, B.C., Canada, 1996.

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Nicholas A. Peppas

1976

Showalter Distinguished Professor of Biomedical Engineering

Degrees

DEng, National Technical University, Athens, 1971

ScD, Massachusetts Institute of Technology, 1973

Interests

Diffusion in Polymers

Polymer / Polymer Adhesion

Polymerization Reaction Engineering

Controlled Release

Biomedical Engineering

Biomedical Polymers

Bioadhesion

Awards and Major Appointments

Visiting Professor, University of Naples, Italy, 1996

Best Paper Award, Materials Division, American Institute of Chemical Engineers, 1995

Best Paper Award, Bioengineering Division, American Institute of Chemical Engineers, 1995

APV Medal for Distinguished Pharmaceutical Contributions, International Pharmaceutical Association, 1995

National Science Foundation Fellowships Panel, 1995

National Science Foundation, Technology for a Sustainable Environmental Panel, 1995

AIChE, Chairman, Committee on Polymers, Area 8a (1995-)

MRS, External Affairs Committee (1995-)

AAPS, Strategic Alliance / Globalization Committee (1995-)

Society for Biomaterials, Chairman, Controlled Release SIG (1995-); Fellows Committee (1995-); Member, Awards and Nominations Committee, 1996

National Institutes of Health, Review Board, March 1996

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 investi-

gated. 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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Dietz, J.E. and N.A. Peppas, "Reaction Kinetics and Chemical Changes During Multifunctional (Meth)acrylate Polymerizations for Highly Crosslinked Information Storage Polymers," *Polymer*, (submitted).

Anseth, K.S., R.A. Scott, and N.A. Peppas, "Effects of Ionization on the Reaction Behavior and Kinetics of Acrylic Acid Polymerization," *Macromolecules*, (submitted).

Sahlin, J.J. and N.A. Peppas, "Monte Carlo Simulations of Grafted Chains at Interfaces," *J. Appl. Polym. Sci.*, (submitted).

Mallapragada, S.K. and N.A. Peppas, "Crystal Unfolding and Chain Disentanglement During Semicrystalline Polymer Dissolution," *AIChE J.*, (submitted).

Editorial Boards

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

Journal of Applied Polymer Science (1976-)

Polymer Gels and Networks (1993-)

Journal of Biomaterials Science, Polymer Edition (1987-)

Biomedical Materials (1985-)

Journal of Controlled Release (1983-)

Advanced Drug Delivery Reviews (1992-)

Tissue Engineering (1994-)

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

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

Tissue Engineering Books, Academic Press (1995-)

Chemical Engineering Progress (1991-93)

Polymer News (1980-92)

Invited Lectures

"Diffusion and Drying Phenomena in Hydrogels: Influence of Gels' Structure and Hydrophilicity," Cygnus, Redwood City, CA, August 31, 1995.

"Multifunctional Methacrylates as Biomaterials in Ocular Applications," Alcon Labs, Ft. Worth, TX, January 23, 1996.

"Hydrogels in Pharmaceutical Applications," B.F. Goodrich, Brecksville, OH, February 1, 1996.

"Mechanistic Aspects of Polymer Dissolution," University of Kentucky, Department of Chemical Engineering, Lexington, KY, February 7, 1996.

"Mechanistic Aspects of Polymer Dissolution," City University of New York, Department of Chemical Engineering, New York, NY, March 18, 1996.

"Poly(vinyl alcohol)-Based Release Systems," ALZA Corporation, Palo Alto, CA, April 30, 1996.

"Intelligent Biomaterials: Scientific Curiosity or Panacea?," Ohio State University, Department of Chemical Engineering, New York, NY, May 2, 1996.

"Diffusion Polymers," University of Naples, Department of Materials Science - Naples, Italy, May 15, 1996.

"Use of Hydrogels in Drug Delivery," University of Naples, Department of Pharmaceutical Chemistry, Naples, Italy, May 21, 1996.

"Swelling-Controlled Release Systems," University of Rome, Department of Pharmaceutical Chemistry, Rome, Italy, May 24, 1996.

Chaired Conferences/ Symposia

Chairman of Session on "Oral Delivery," First Spanish Portuguese Conference on Controlled Drug Delivery, Santiago de Compostela, Spain, September 1995.

Organizer and Chairman of Sessions on "Diffusion in Polymers," AIChE Meeting, Miami Beach, FL, November 1995.

Chairman of Session on "Drug Delivery," World Congress of Biomaterials, Toronto, Ontario, May 1996.

Chairman of Session on "Hydrogels," 23rd International Conference on Controlled Release of Bioactive Materials, Kyoto, Japan, July 1996.

Meeting Presentations

"Fickian and non-Fickian Diffusion in Swellable Gels," 36th IUPAC Microsymposium on High-Swelling Gels, Prague, Czech Republic, July 10, 1995.

"Transport in Hydrophilic Polymer Gels: Applications in Controlled Release," 22nd International Symposium of Controlled Release of Bioactive Materials, Seattle, WA, August 1, 1995.

"Effect of Dissolution on Lamellar Thickness Distribution of Semi-Crystalline Poly(vinyl alcohol)," Annual ACS Meeting, Chicago, IL, August 24, 1995

"Development of a Dissolution-controlled, Zero-order Release, Drug Delivery System," Annual ACS Meeting, Chicago, IL, August 21, 1995.

"Recent Developments in Insulin Delivery and Control Using Hydrogel Systems," Spanish Portuguese Conference on Controlled Drug Delivery, Santiago de Compostela, Spain, September 25, 1995

"Chain Disentanglement and Reptation Mechanisms During Polymer Dissolution," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"A New Model for Dissolution of Semicrystalline Polymers," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"Transport in Swellable Polymer Systems for Controlled Drug Release," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"Rate Behavior in Solution Polymerization of Acrylic Acid," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"Swelling / Deswelling Behavior in pH-Responsive Hydrogels of Ethylene Glycol Poly(Methacrylic acid) Copolymers," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"Glucose-responsive Gels for the Release of Insulin," Annual AIChE Meeting, Miami Beach, FL, November 13, 1995.

"Intelligent Hydrogel Systems for Protein and Drug Release with Feedback Control," 3rd US-Japan Symposium on Drug Delivery Systems, Maui, HI, December 18, 1995.

"A Self-Consistent Diffusivity Approach to Understand Polymer Dissolution," American Physical Society Meeting, St. Louis, MO, March 19, 1996.

"Modeling of Dissolution of Semicrystalline Polymers," American Physical Society Meeting, St. Louis, MO, March 19, 1996.

"Modification of Drug Release Profiles and Swelling Behavior in Poly(vinyl alcohol) due to the Presence of a Crystalline Phase," American Chemical Society Meeting, New Orleans, LA, March 26, 1996.

"On the Mechanisms of Water Transport and Drug Release from Swellable Hydrogels," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Solid State NMR Spectroscopy for Characterization of Acrylate Reaction," American Chemical Society Meeting, New Orleans, LA, March 26, 1996.

"Radiation Crosslinked Poly(ethylene oxide) Hydrogels Show Insignificant Diffusional Screening Effects," American Chemical Society Meeting, New Orleans, LA, March 26, 1996.

"An Experimental Study of Acrylic Acid Crosslinking Polymerizations," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Molecular Aspects of the Swelling Behavior of Interpolymer Complexing Hydrogels," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Glucose-responsive Complexation Hydrogels," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Kinetics of UV Polymerization of Acrylic Acid," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Release of Insulin from Glucose-Sensitive Hydrogel," American Chemical Society Meeting, New Orleans, LA, March 27, 1996.

"Design of New Biomaterials for Drug Delivery: Tailoring the Structure to Specific Delivery Needs and Release Requirements," European Course on New Forms and New Routes of Administration of Drugs, Parma, Italy, March 30, 1996.

"Mucoadhesive PVA Hydrogels for Release of Wound Healing Drugs," Fifth World Biomaterials Congress, Toronto, Canada, June 1, 1996.

Doraiswami Ramkrishna

1976

Harry Creighton Peffer Distinguished Professor of Chemical Engineering

Degrees

BS, University of Bombay, 1960

Ph.D., University of Minnesota, 1965

Interests

Chemical Reaction Engineering

Dispersed Phase Systems

Biochemical Engineering

Applied Mathematics

Awards and Major Appointments

Elected Fellow of the American Institute for Medical and Biological Engineering

Visiting Professor, P. R. China (Zhejiang and East China) Universities, November 28-December 13, 1995

Research Areas

Chemical Reaction Engineering: Spatial pattern formation has been investigated in packed bed 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 by introducing multiple feeds as a start-up strategy. Recent investigations of the stability of pattern *classes* which assure product quality have set the proper scenario for future investigation of the control of patterned steady states in catalytic reactors. With Professor Delgass, an experimental program is being initiated to study the development of patterns using NMR techniques.

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.

Other activities include population balance modeling of particle size distributions in precipitation and crystallization processes, particularly in small systems such as emulsion droplets and reverse micelles. Stochastic population balances have been applied to calculate not only average size distributions but also fluctuations about the mean.

Efficient strategies have been developed for numerical solutions of discretized population balance equations which compute selected properties of the system accurately with very coarse discretizations that may be ideally suited for applications to model-based control of particle size distributions.

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. A new approach is under investigation to hindered creaming of droplets based on a combination of population balance and experimental measurement of number densities at the inlet and outlet of a continuous, vertical column. An experimental study of coalescence in the cream layer has been initiated.

Biochemical Engineering: A novel class of cybernetic models have been developed for describing microbial systems in mixed substrate environments which can describe contrasting situations of sequential as well as simultaneous uptakes substitutable substrates also accounting for dependence on preculturing of the organisms. Nonlinear mathematical analysis revealing the models' full multiplicity and stability structure which govern 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 rates 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.

A self-similar theory of microbial populations was advanced to make quantitative interpretations about processes in single cells from dynamic population data obtained from flow cytometers. This theory is presently under investigation with simulated data towards establishing strategies for treatment of cytometric data.

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. A new stochastic bridge process simulation technique has been developed which exactly takes into account the probability of polymer conformations in an external field as specified by statistical mechanics.

Publications

Ramkrishna, D., A Sathyagal, and G. Narsimhan, "Analysis of Dispersed Phase Systems. Fresh Perspective," *AIChE J., 41,* 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.

Gandhi, K.S., R. Kumar, and D. Ramkrishna, "Some Basic Aspects of Reaction Engineering of Precipitation Processes," *Ind. & Eng. Chem.*, (BSL Issue), *34*, 3223-3230, 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.*, 51, 1377-1391, 1996.

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

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

Kumar, S., G. Narsimhan and D. Ramkrishna, "Coalescence in Creaming Emulsions. Existence of a Creaming-Free Zone," *Ind. & Eng. Chem. Res. (Ruckenstein issue)*, (in press).

Kumar, S. and D. Ramkrishna, "On the Solution of Population Balance Equations by Discretization I." *Chem. Eng. Sci.*, *51*, 1311-1332, 1996.

Kumar, S. and D. Ramkrishna, "On the Solution of Population Balance Equations by Discretization II," *Chem. Eng. Sci., 51*, 1333-1342, 1996.

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

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

Lam, A., A. Sathyagal, S. Kumar and D. Ramkrishna, "On the Maximum Stable Drop Diameter in Stirred Dispersions," *AIChE J., 42*, 1547-1552, 1996.

Narang, A., A.E. Konopka and D. Ramkrishna, "New Patterns of Mixed Substrate Utilization During Batch Growth of *Escherichia coli," Biotech. & Bioeng.*, (submitted).

Narang, A., A.E. Konopka and D. Ramkrishna, "The Dynamics of Microbial Growth in Mixtures of Substrates in Batch Reactors," *J. of Theoretical Biology,* submitted.

Trinh, S. and D. Ramkrishna, "Spatiotemporal Patterns in a Catalytic Reactor," *Can. J. Chem. Eng.,* (submitted).

Narang, A., A.E. Konopka and D. Ramkrishna, "Dynamic Analysis of the Cybernetic Model for Diauxic Growth," *Chem. Eng. Sci.*, (in press).

Ramakrishna, R., A.E, Konopka, and D. Ramkrishna, "Microbial Growth on Substitutable Substrates. Characterizing the Consumer Resource Relationship," *Biotech. Prog.*, (in press).

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

Gandhi, K.S., R. Bandopadhyay, R. Kumar and D. Ramkrishna, "Particle Size During Precipitation in Reverse Micelles," *Langmuir*, (submitted).

Invited Lectures

Three lectures on population balances, Department of Chemical Engineering, Indian Institute of Science, Bangalore, July 1995.

Four lectures on "Modeling of Microbiol Processes," as World Bank sponsored visitor of P.R. China, Department of Chemical Engineering, Zhejiang University, December 4-9, 1995.

Two lectures on "Modeling of Microbial Processes," Laboratory of Bioreactor Engineering, East China University, December 11, 12, 1995.

Plenary lecture on "The Packed Bed Reactor. A Modeler's Delight," Chemcon 95: joint-meeting AIChE and IIChE (Indian Institute of Chemical Engineers), December 27-29, 1995.

Meeting Presentations

Ramkrishna, D., and S. Trinh, "Unsteady Spatio-Temporal Patterns in Catalytic Reactors," 2nd International Conference on Unsteady State Processes in Catalysis, St. Louis, MO, September 10-14, 1995.

Pirog, T., S. Kumar, G. Narsimhan and D. Ramkrishna, "A New Procedure for Hindered Creaming Velocity Determination for Polydisperse Dispersions," Paper No. 103g, AIChE Annual Meeting, 1995, Miami Beach, FL, November 12-17, 1995.

Kumar, S. and D. Ramkrishna, "A General Discretization Technique for Solving Population Balance Equations Involving Bivariate Distributions," Paper No. 139c, AIChE Annual Meeting, 1995, Miami Beach, FL, November 12-17, 1995.

Starry, A., J. Caruthers and D. Ramkrishna, "Nonlinear Fluctuating Hydrodynamics of a Viscoelastic Fluid," Paper No. 169a, AIChE Annual Meeting, 1995, Miami Beach, FL, November 12-17, 1995.

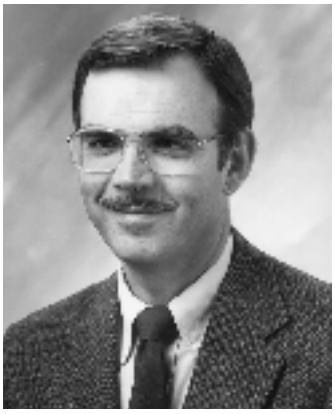
Trinh, S. and D. Ramkrishna, "Pattern Formation in Packed Bed Catalytic Reactors," Paper No. 170g, AIChE Annual Meeting, 1995, Miami Beach, FL, November 12-17, 1995.

Ramakrishna, R., A. Konopka and D. Ramkrishna, "Cybernetic Modeling of Microbial Growth on Mixed Substrates. Application to Bioremediation Strategies," Paper No 218e, AIChE Annual Meeting, 1995, Miami Beach, FL, November 12-17, 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

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

Computer Applications in Engineering Education, Editorial Board, 1992-

Council for Chemical Research, Member, Governing Board, 1994-1997; Chair, International Committee, 1993-

Kirkpatrick Chemical Engineering Achievement Award, Board of Judges, 1991- ; Chair, 1995

Advisory Board, Department of Chemical Engineering, Carnegie-Mellon University, 1991-

Best Paper Award, Computers & Chemical Engineering, Vol. 18, 1994

Publications

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.

Reklaitis, G.V., "Scheduling Approaches for the Batch Process Industries," *ISA Transactions*, 34, 349-358, 1995.

Jayakumar, S. and G.V.Reklaitis, "Chemical Plant Layout via Graph Partitioning, Part II: Multiple Levels," *Computers & Chem. Engng.,* 20, 563-778, 1996.

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*, 20, 821-844, 1996.

Jayakumar, S., R.G. Squires, G.V.Reklaitis, P.K. Andersen and B.K. Dietrich, "The Purdue-Dow Styrene Butadiene Polymerization Simulation," *J. Eng. Educ.* 84, 271-277, 1995.

Mockus, L. and G.V. Reklaitis, "A New Global Optimization Algorithm for Batch Process Scheduling," in *State of the Art in Global Optimization,* C.A. Floudas and P.M. Pardalos (eds), Kluwer Academic Publishers, pp. 521-538, 1996.

Subrahmanyam, J.F. Pekny and G.V. Reklaitis, "Decomposition Approaches to Batch Design and Planning," I&EC Research, 35, 1866-1876, 1996.

Squires, R.G., K. Kuriyan, S. Jayakumar, G.V.Reklaitis, M. Evans, B. Morrato and R. Gutwein, "The Procter & Gamble Decaffeination Project - A Mulitmedia Instruction Module," *Comput. Appl. Engr. Education*, 1996 (in press).

Mockus, L. and G.V. Reklaitis, "Mathematical Programming Formulation for Scheduling of Batch Operations based on Nonuniform Time Discretization," *Computers & Chem. Engng.,* 1996 (in press).

Reklaitis, G.V. and L.B. Koppel, "Role and Prospects for Intelligent Systems in Integrated Process Operations," *Intelligent Systems in Process Engineering,* G. Stephanopoulos, V. Venkatasubramanian and J. Davis (eds), CACHE-AIChE, 1996.

Bassett, M., J.F. Pekny and G.V. Reklaitis, "Decomposition Techniques for the Solution of Large Scale Scheduling Problems Associated with Batch Chemical Processes," *AIChE J.* (accepted).

Invited Lectures

"Role and Prospects for Intelligent Systems in Integrated Process Operations," International Symposium on Intelligent Systems in Process Engineering," Snowmass, CO, July 1995

"The Role of Optimization Methods in Process Systems Engineering," IFORS Conference on OR and Engineering Design, St. Louis, MO, October 1995

Chaired Confrences/ Symposia

World-wide Industry-University-Government Research Collaboration Models in the Chemical Sciences and Engineering, CCR-NSF Workshop, Pittsburgh, PA, October 7, 1995.

Globalization of Research, CCR Annual Meeting, October 8-10, 1995, Plenary session chair.

6th European Symposium on Computer Aided Process Engineering (ESCAPE6), Rhodes, Greece, May 1996, Plenary session co-chair.

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

Meeting Presentations

"Bayesian Approach in Batch Process Scheduling," paper WA1.3., IFORS Conference on Operation Research and Engineering Design, St. Louis, MO, 1995.

"Design of Optimal Feed and Reflux Policy for Multicomponent Reactive Distillation," paper No. 21b, AIChE Annual Meeting, Miami Beach, FL, November 1995.

"A Bayesian Approach in Batch/Semicontinuous Process Scheduling: Computational Comparisons," paper No. 174c, AIChE Annual Meeting, Miami Beach, FL, November 1995.

"Intelligently Utilizing Process Recipes within Scheduling Heuristics," paper No. 177d, AIChE Annual Meeting, Miami Beach, FL, November 1995.

"Campaign Optimization of Multicomponent Reactive Batch Distillation," paper No. 83f, AIChE National Meeting, New Orleans, LA, February 1996.

"An Integrated Approach to Economic and Environmental Issues in Design of Batch Chemical Process," paper No. 87b, AIChE National Meeting, New Orleans, LA, February 1996.

"Continuous Time Representation in Batch/Semicontinuous Process Scheduling: Randomized Heuristics Approach," 6th European Synposium on Computer Aided Process Engineering (ESCAPE6), Rhodes, Greece, May 1996.

Eva Sevick-Muraca

1994

Associate Professor

Degrees

National Institutes of Health Post Doctoral Fellow in Biophysics and Biochemistry

University of Pennsylvania, 1989-1991

PhD, Carnegie Mellon University, 1989

MS, University of Pittsburgh, 1985

BS, University of Pittsburgh, 1983

Interests

Biomedical Optical Diagnostics

Optical Spectroscopy and Imaging in Random Media

Process Monitoring for Particle Size Control Using Measurements of Photon Migration

Inverse Problems in Optical Engineering

Awards and Major Appointments

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

National Science Foundation Young Investigator Award, 1993-1998

Whitaker Foundation Research Award, 1991-1994

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

Laboratory for Fluorescence Dynamics Advisory Board, University of Illinois at Urbana-Champaign Department of Physics, October 1995-October 1996

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

National Institutes of Health Review Panel, Special Study Sections, 1993-present

*National Academy of Engineering, Frontiers of Engineering Symposium, Irvine, CA, September 1995

*Member of industrial research consortia: 1.Measurement and Control Engineering Center, University of Tennessee (Knoxville), National Science Foundation Industrial/University Cooperative Research Center, September 1993-present. 2.National Science Foundation I/UCRC for Industrial Pharmacy, Purdue University, May 1995-present

Research Areas

The recent advances in laser diode technology and photodetection make possible the development of non-invasive, near-infrared, sensors for diagnosis in biotechnology, clinical medicine, and process monitoring. Currently near-infrared technologies are based upon measuring the time-averaged attenuation and / or backscatter for determination of particle size distributions, tissue hemoglobin saturation, and / or (bio-) chemical compositions. Unfortunately, the intense and variable scattering properties of the pertinent (on-line) systems of interest make the inverse problem intractable, thereby requiring empirical calibrations. When employed in dynamic systems, these empirical calibrations fail and the predictive power of photonic sensors is lost.

In the research conducted in the Photon Migration Laboratory, instead of measuring the amount of light transmitted or backscattered from optically dense systems, Professor Sevick's research team measures migration characteristics: Specifically, the distribution of picosecond "time-of-flights" for photons transmitted across several centimeters of a multiply scattering medium, whether that medium be in vivo or ex vivo tissues, cured ultrahigh molecular weight polyethylenes, latex suspensions, or lipid emulsions. For media composed of non-interacting, randomly distributed scatters, the diffusion approximation to the radiative transfer equation is employed in order to determine scattering and absorption cross sectional areas as well as fluorescence yield and lifetimes, when appropriate. For samples composed of interacting, packed scatters (such as powders), the problem is more complex requiring analysis of structure factors and correction factors for deviation of local electric fields due to nearest neighbor scatterers. Three applications of time-dependent light propagation measurements are the subject of research expenditures in the Photon Migration Laboratory:

Application#1: Photon migration imaging for breast cancer screening

In recent years, the early detection of preclinical breast cancer has been proposed as the most beneficial tool against a disease which one in eight women in the United States will encounter. 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. In this population, the benefit achieved from x-ray mammography screening is outweighed by the small yet finite risk associated with repeated doses of x-irradiation. Consequently, a large unserved population who are at risk for the disease do not have a dependable screening tool.

In Professor Sevick's research program, a biomedical optical imaging device which is dependent upon the radiative scatter for image formation is under development. The new imaging technique, called Photon Migration Imaging (PMI), is not compromised by tissue scatter, but is enhanced by it. Essentially, the frequency-domain technology consists of illuminating a tissue with near-infrared light whose intensity is sinusoidally modulated at MHz frequencies. Using a CCD camera and image intensifier operated in homodyne mode, 512x512 measurements of phase-shift and amplitude modulation or re-emitted, multiply scattered light are made a various modulation frequencies. Using this system, acquisition is rapid providing a sufficiently large data set for input into the inverse algorithm. The inverse algorithm consists of an it-

erative approach to vary optical properties at individual positions with the tissue until the measurements of phase-shift and amplitude modulation match those predicted by the optical diffusion equation. With industrial and federal support of this research program, Professor Sevick's team is developing the tools and theory for the realization of a safe, non-ionizing method for detecting breast cancer in population unserved by current modalities.

Application #2: Lifetime-based spectroscopy in tissues and other random media using fluorescent probes

The development of stable optical fluorescent probes promises non-invasive, diagnostic spectroscopy for tissues and other random media. For example, glucose does not exhibit a significant NIR spectrum for non-invasive measurement via photon migration techniques. Yet there are stable fluorescent compounds whose re-emission kinetics are directly related to local glucose concentrations -- potentially enabling a non-invasive glucometer for diabetics without the need to draw blood. 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.

In the Photon Migration Laboratory, established techniques of frequency-domain measurement of optical probe lifetimes are coupled with a simple algorithm for excitation and fluorescent light propagation in tissues in order to quantitate metabolite and other (bio-) chemical concentrations from fluorescent re-emissions. The fluorescent lifetime-based approach differs from fluorescent intensity measurements in that calibration is not necessary and deconvolution of tissue optical properties is not required. Herein, the lifetime is defined as a mean time between the absorption of an excitation photon and the re-emission of a fluorescent one. Using finite element solutions to the coupled integral-differential equations for excitation and fluorescent light propagation, Professor Sevick's research team has shown that photon migration times are readily accounted for by simple "referencing" measurements. These coupled studies of photon migration and fluorescence / phosphorescence kinetics are imperative for the successful development of optical probes as diagnostic tools in biology, medicine, and process monitoring. This work has coupled directly into research on fluorescence lifetime-based optical imaging, a recent discovery made in the Photon Migration Laboratory at Purdue University.

Application #3: Process monitoring using measurements of photon migration

The measurement of critical variables for chemical and pharmaceutical processes involving polymer melts, powders, polydisperse slurries, dispersed phases 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 to which their calibration is based.

In research conducted in the Photon Migration Laboratory, we are developing methods for determining the concentration, particle size distribution, and concentration of chemical constituents from frequency-domain measurements conducted on-line. Frequency-domain techniques consist of delivering intensity modulated light to the process stream and collecting the multiply scattered light through fiber optic couplings. Fast-electro-optics coupled with a model based analysis of signals provides self-calibrating measurements of scattering and absorption — quantities that are inverted into industrially relevant parameters for control. Inverse solutions for determination of particle or dispersed phase size distribution are studied along with multivariate analyses to assess resonances to chemical products and reactants.

Publications

Sevick-Muraca, E.M. and D. Benaron (Eds.), *OSA Trends in Optics and Photonics on Biomedical Optical Spectroscopy and Diagnostics*, Optical Society of America, Washington, DC, 1996.

Hutchinson, C.L., T.L. Troy and E.M. Sevick-Muraca. "Fluorescence-lifetime determination in tissues and other random media from measurement of excitation and emission kinetics," *Applied Optics*, 35: 2325-2332, 1996.

Troy, T.L., D.L. Page and E.M. Sevick-Muraca, "Optical properties of normal and diseased breast tissues: prognosis for optical mammography," *J. Biomedical Optics,* 1:1-19, 1996 (invited).

Richards-Kortum, R. and E.M. Sevick-Muraca, "Quantitative optical spectroscopy for tissue diagnostics," *Annual Review of Physical Chemistry*, 47:555-606, 1996.

Sevick-Muraca, E.M., C.L. Hutchinson and T.L. Troy, "Fluorescence-lifetime based sensing in tissues and other random media with measurement of photon migration," in *Analytical use of fluorescent probes in oncology*, Ed. E. Kohen, Plenum Press, New York, 1996.

Paithankar, D.Y., A.U. Chen, B.W. Pogue and M.S. Patterson, "Imaging of fluorescent yield and lifetime from multiply scattered light reemitted from tissues and other random media," submitted, 1996.

Sevick-Muraca, E.M., Paithankar, D.Y., C.L. Hutchinson and T.L. Troy, "Analysis of photon migration for optical diagnosis," Proc. Soc. Photo-Opt. Instrum. Eng., 2680: 114-123, 1996 (invited).

Paithankar, D.Y., A. Chen and E.M. Sevick-Muraca, "Fluorescence yield and lifetime imaging in tissues and other scattering media," Proc. Soc. Photo-Opt. Instrum. Eng., 2679: 162-175, 1996.

Sevick-Muraca, E.M., C.L. Hutchinson and D.Y. Paithankar, "Optical Tissue Biodiagnostics Using Fluorescence Lifetime" *Optics and Photonics News*, 7:25-28, 1996.

Sevick-Muraca, E.M. and C.L. Hutchinson "Probability description of fluorescent and phosphorescent signal generation in tissues and other random media," Proc. Soc. Photo-Opt. Instrum. Eng., 2387: 274-283, 1995.

Burch-Hutchinson, C.L., and E.M. Sevick-Muraca "Fluorescence spectroscopy and imaging in random media," Proc. Soc. Photo-Opt. Instrum. Eng., 2389: 62-70, 1995.

Editorial Boards

Photochemistry and Photobiology (Associate Editor), 1995-1999.

Applied Optics (Special Topics Editor: special issue on fluorescence diagnostics in tissues), 1996.

Journal of the Optical Society of America A, (Special Topics Editor: special issue "Diffusing photons in random media"), 1996.

Invited Lectures

"Near-infrared biomedical optical imaging with measurements of photon migration," Progress in Electromagnetics Research Symposium," Seattle, WA, July 1995.

"Measurement of particle size distributions with photon migration," DuPont Engineering Research, Wilmington, DE, August 1995

"Measurements of time-dependent fluorescent photon migration for tissue spectroscopy and imaging," Optical Society of America National Meeting, Portland, OR, September 15, 1995.

"Lifetime-based spectroscopy in tissues," NATO Advanced Research Workshop: Analytical use of fluorescent probes in oncology, Miami Beach, FL, October 17, 1995.

"Photon migration measurements for process monitoring in particulate processes," Eli Lilly Corporate Center, Corporate Process Automation, Indianapolis, IN, October 1995.

"Photon migration measurements for process monitoring, biodiagnostics, and biomedical optical imaging," James and Catherine Pattern Chemical Engineering Seminar Series, Department of Chemical Engineering, University of Colorado, Boulder, CO, November 9, 1995.

"Biophotonics for tissue diagnostics," Laser Focus World's Medical Laser Marketplace seminar, San Jose, CA, January 30, 1996.

"Chemical based sensing via fluorescent lifetime measurements in situ," American Society for Neurochemistry, 27th Annual Meeting, Philadelphia, PA, March 6, 1996.

"Non-invasive optical biodiagnostics with measurement of photon migration," Department of Biomedical Engineering, Northwestern University, Chicago, IL, April 2, 1996.

"Time-dependent measurements of multiply scattered light for process monitoring," Hercules Chemical Company, Ninth Annual Process Analytics Symposium, Wilmington, DE, May 23, 1996.

"Photon migration measurements for on-line micron and submicron particle sizing: research and development," Air Products, Allentown, PA, June 27, 1996.

Chaired Conferences/ Symposia

Optical Society of America Topical Meeting for Biomedical Optical Spectroscopy and Diagnostics, Orlando, FL, March 1996 (program chair).

"New Directions for Time-Dependent Measurements of Photon Migration," in "Future Directions for Lasers in Medicine and Surgery," Engineering Foundation Conferences, Snowbird, UT, July 11-16, 1995 (program co-chair).

"Advances in Laser and Light Spectroscopy to Diagnose Cancer and other Diseases III: Optical Biopsy" Biomedical Optics Meeting, The International Society for Optical Engineering, San Jose, CA, February 1996 (program planning committee).

"Optical techniques in Chemical Engineering," American Institute of Chemical Engineers, Miami, FL, November, 1995 (session chair).

Meeting Presentations

Sevick-Muraca, E.M., Troy, T.L., Hutchinson, C.L., Nelson, L., Smith, J. and L. Page, "Photon migration imaging for breast cancer screening," Bioengineering Conference, The American Society of Mechanical Engineers, Beaver Creek, CO, July 1995.

Sevick-Muraca, E.M., Hutchinson, C.L. and T.L. Troy, "Lifetime-based spectroscopy for tissue diagnostics," Bioengineering Conference, The American Society of Mechanical Engineers, Beaver Creek, CO, July 1995.

Sevick-Muraca, E.M. "On the origin of optical signals re-emitted from tissues," in Future Directions for Lasers in Medicine and Surgery, Engineering Foundation Conference, Snowbird, UT, July 1995.

Paithankar, D., Kao, J., and E. M. Sevick-Muraca, "Particle size distribution via solution of the inverse problem of multi-wavelength scattering coefficient measurements," 26th Annual Meeting of the Fine Particle Society, Chicago, IL, August 1995.

Pierce, J., Paithankar, D., Hutchinson, C., and E.M. Sevick-Muraca, "Particle size measurement in suspesions using frequency-domain photon migration measurements," 26th Annual Meeting of the Fine Particle Society, Chicago, IL, August 1995.

Hutchinson, C.L., Troy, T.L., Paithankar, D., and E.M. Sevick-Muraca, "Lifetime-based sensing in scattering media," Biomedical Engineering Society Annual Meeting, Boston, MA, October 1995.

Troy, T.L., Nelson, L., Paithankar, D., and E.M. Sevick-Muraca, "Photon migration imaging for breast cancer detection," Biomedical Engineering Society Annual Meeting, Boston, MA, October 1995.

Paithankar, D., J. Pierce, K. Yasuda, C. Hutchinson, D. Taylor and E.M. Sevick-Muraca, "Particle size measurement in suspensions and powders using frequency-domain photon migration measurement," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, FL, November 1995.

Troy, T.L., L. Nelson, D. Paithankar and E.M. Sevick-Muraca, "Photon Migration for Breast Cancer Detection," Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, FL, November 1995.

Troy, T.L., L. Nelson, C.L. Hutchinson and E.M. Sevick-Muraca, "Investigation of exogenous contrast agents for biomedical optical imaging," Biomedical Optical Spectroscopy and Diagnostics, Sevick-Muraca and Benaron (Eds.), Optical Society of America, March 1996.

Hutchinson, C.L., T.L. Troy and E.M. Sevick-Muraca, "Fluorescence lifetime spectroscopy and imaging in random media," Sevick-Muraca and Benaron (Eds.), Optical Society of America, March 1996.

Troy, T.L. and E.M. Sevick-Muraca, "Optical Properties of Normal and Diseased Breast Tissue," Biomedical Optical Spectroscopy and Diagnostics, Sevick-Muraca and Benaron (Eds.), Optical Society of America, March 1996.

Pierce, J.E. and E.M. Sevick-Muraca, "Particle sizing from multi-wavelength frequency-domain measurements of photon migration." Laser Applications to Chemical and Environmental Analysis, Optical Society of America Topical Meeting, March 1996.

Kao, J. and E.M. Sevick-Muraca, "Particle sizing using time-domain techniques of photon migration," Laser Applications to Chemical and Environmental Analysis, Optical Society of America Topical Meeting, March 1996.

Paithankar, D.Y. and E.M. Sevick-Muraca, "Fluorescence lifetime imaging with frequency-domain photon migration measurement," Biomedical Optical Spectroscopy and Diagnostics, Sevick-Muraca and Benaron (Eds.), Optical Society of America, March 1996.

Paithankar, D.Y. and E.M. Sevick-Muraca, "Fluorescence lifetime imaging for biodiagnostics," Optical Society of America, Conference on Lasers and Electro-Optics, Anaheim, CA, June 1996.

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

Jayakumar, S., R.G. Squires, G.V. Reklaitis, P. K. Andersen and B.K. Dietrich, "The Purdue-Dow Styrene-Butadiene Polymerization Simulation," *J. Eng. Educ.,* Vol. 84, No. 3, pp. 271-277, 1995.

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

Squires, R.G., K. Kuriyan, S. Jayakumar, G.V. Reklaitis, M. Evans, B. Morrato and R. Gutwein, "The Procter & Gamble Decaffeination Project - A Multimedia Instruction Module," *Computer Applications in Engineering Education,* in press, 1996.

Christos G. Takoudis

1981

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

Partial Oxidation on Catalytic Surfaces

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 funda-

mental questions like the ones mentioned above. In fact, chemical engineers 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 of 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., 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. 99*, 4599-4608, 1995.

Tolia A.A., C.T. Williams, M.J. Weaver and C.G. Takoudis, "Surface-Enhanced Raman Spectroscopy as an In-Situ Real-Time Probe of Catalytic Mechanisms at High Gas Pressures: The NO-H_2 Reaction on Rhodium," *Langmuir 11*, 3438-3446, 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, 215-218, 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, 164-167, 1995.

Hase R., C.G. Takoudis and R. Uzsoy, "Alternative Facility Layouts for Semiconductor Wafer Fabrication Facilities," *Proceedings of Seventeenth International Electronics Manufacturing Technology Symposium*, Austin, TX, 384-388, 1995.

Chen S., R.C. Hase, K. Mordaunt, R. Uzsoy and C.G. Takoudis, "Relationships Between Process Fundamentals, Facility Design, and Production Control of Semiconductor Manufacturing Systems," *Proceedings of Microelectronic Manufacturing 1995 Symposium*, Austin, TX, 168-178, 1995.

Lee I-M., W.-C. Wang, G.W. Neudeck and C.G. Takoudis, "Kinetics and Modeling of Low Pressure Chemical Vapor Deposition of $Si_{1-x}Ge_x$ Epitaxial Thin Films," *Chem. Eng. Sci. 51*, 2681-2686, 1996.

Lee I-M., G.W. Neudeck and C.G. Takoudis, "Low Pressure Chemical Vapor Deposition of Epitaxial Silicon-Germanium, Epitaxial Silicon and Poly-Silicon," *Electrochem Soc. 96-5*, 107-112, 1996.

Panczyk C. and C.G. Takoudis, "*In Situ* Infrared Emission Spectroscopy During Silicon Chemical Vapor Deposition," *Electrochem Soc. 96-5*, 183-188, 1996.

Williams C.T., A.A. Tolia A.A., M.J. Weaver and C.G. Takoudis, "Surface-Enhanced Raman Spectroscopy as an In-Situ Real-Time Probe NO Reduction over Rhodium at High Gas Pressures," *Chem. Eng. Sci. 51*, 1673-1682, 1996.

Lee I.-M. and C.G. Takoudis, "Process-Property Relationships in $Si_{1-x}Ge_x$ Chemical Vapor Depiosition - Thermodynamic and Kinetic Studies," *J. Electrochem. Soc. 143*, 1719-1726, 1996.

Lee I-M., G.W. Neudeck and C.G. Takoudis, "Low Pressure Chemical Vapor Deposition of Epitaxial Silicon-Germanium, and Epitaxial Silicon," *Electrochem Soc. 96-1*, 911-912, 1996.

Panczyk C. and C.G. Takoudis, "*In Situ* Emission IR Spectroscopy During Silicon CVD," *Electrochem Soc. 96-1*, 921-922, 1996.

Williams C.T., A.A. Tolia, H. Chan, 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 Platinum and Palladium," *J. Catal.*, in press, 1996.

Meeting Presentations

"Alternative Facility Layouts for Semiconductor Wafer Fabrication Facilities," Seventeenth International Electronics Manufacturing Technology Symposium, Austin, TX, October 2-4, 1995.

"Relationships Between Process Fundamentals, Facility Design, and Production Control of Semiconductor Manufacturing Systems," Microelectronic Manufacturing 1995 Symposium, Austin, TX, October 25-26, 1995.

"Surface-Enhanced Raman Spectroscopy as an *In Situ* Real-Time Probe of Catalytic Mechanisms at High Gas Pressures: The $NO-H_2$ Reaction on Rhodium," Annual Meeting, AIChE, Miami Beach, FL, November 12-17, 1995.

"Fundamental Studies of Hydrogen Passivated Silicon Surfaces Prepared by a Two-Step HF Wet Chemical Etching Method," Annual Meeting, AIChE, Miami Beach, FL, November 12-17, 1995.

"*In Situ* Analysis of Adsorbed and Reaction Intermediates During the Chemical Vapor Deposition of Silicon Thin Films Using Emission Infrared Spectroscopy," Annual Meeting, AIChE, Miami Beach, FL, November 12-17, 1995.

"Determining Thickness and Composition of $Si_{1-x}Ge_x$ Films by Ellipsometry," Annual Meeting, AIChE, Miami Beach, FL, November 12-17, 1995.

"Kinetics and Modeling of Low Pressure Chemical Vapor Deposition of $Si_{1-x}Ge_x$ Epitaxial Thin Films," Fourteenth International Symposium on Chemical Reaction Engineering, Brugge, Belgium, May 5-8, 1996.

"Surface-Enhanced Raman Spectroscopy as an In-Situ Real-Time Probe NO Reduction over Rhodium at High Gas Pressures," Fourteenth International Symposium on Chemical Reaction Engineering, Brugge, Belgium, May 5-8, 1996.

"Low Pressure Chemical Vapor Deposition of Epitaxial Silicon-Germanium, Epitaxial Silicon and Poly-Silicon," Thirteenth International Conference on Chemical Vapor Deposition, Los Angeles, CA, May 5-10, 1996.

"*In Situ* Infrared Emission Spectroscopy During Silicon CVD," Thirteenth International Conference on Chemical Vapor Deposition, Los Angeles, CA, May 5-10, 1996.

Invited Lectures

"Relationships among Microelectronic Material Properties, Processing Environments, and Structure for Si, and SiGe in Two and Three-Dimensional Integration," National Centre for Scientific Research 'Demokritos', Athens, Greece, July 7, 1995.

"Real-Time In Situ Probing of Adsorbed Species and Intermediates in Heterogeneous Catalytic Reactors," Department of Chemical Engineering, National Technical University of Athens, Athens, Greece, July 10, 1995.

"Heterogeneous Catalysis - *In Situ* Real-Time Studies at High Gas Pressures," Mobil, Paulsboro, NJ, December 4, 1995.

"*In Situ* Real-Time Studies of Heterogeneous Reaction Systems at High Gas Pressures," Department of Chemical Engineering, University of Illinois, Chicago, IL, January 19, 1996.

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 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 interations between the depositing particles and the surface and preadsorbed particles.

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

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., 103*, 1607, 1995.

Talbot, J., "Time-Dependent Desorption: A Memory Function Approach,"*Adsorption, 2*, 89, 1996.

Bereolos, P., J. Talbot and K.C. Chao and J. Talbot, "Simulation of Free Energy in the NPT Ensemble without Particle Insertion," *Mol. Phys*. in press, 1996.

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 53*, 785, 1996.

Kivelson, D., J. Talbot, G. Tarjus and J. Variyar, Response to "Comment on 'Negative Velocity Correlaton in Hard Sphere Fluid,'" *J. Chem. Phys., 103*, 9514, 1995

Talbot, J., "Molecular Thermodynamics of Binary Mixture Adsorption:A Scaled Particle Theory Approach," *J. Chem. Phys*., (submitted).

Invited Lectures

"Theory and Applications of Protein Adsorption," Department of Chemical Engineering, University of Michigan, October 1995.

"Molecular Thermodynamics of Multicomponent Adsorption," Laboratoire de Physique Theorique des Liquides, Université Pierre et Marie Curie, Paris, France, July 1996.

Meeting Presentations

"Effects of Protein Adsorption Kinetics at Liquid-Solid Interfaces: Simulation and Statistical Mechanics." *P. R. Van Tassel*, P. Viot, G. Tarjus and J. Talbot, AIChE Annual Meeting, Miami, FL, November 1995.

"Structure and Elastic Properties on Nanometer-Size Metal Clusters." *D. Paithankar*, J. Talbot and R. P. Andres, AIChE Annual Meeting, Miami, FL, November 1995.

"Adsorption Studies of a Mixture on Chemically Modified Porous Media." K. Raghavan and *J. Talbot,* AIChE Annual Meeting, Miami, FL, November 1995.

George T. Tsao

1974

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

Degrees

BS, National Taiwan University, 1953

MS, University of Florida, 1956

PhD, University of Michigan, 1960

Interests

Biochemical engineering

Renewable resource utilization

Publications

Zheng, Y., X. Ting, P. Cen, C. W. Yang, and G. T. Tsao, "Lactic Acid Fermentation and Adsorption on PVP," *Applied Biochem. Biotechnology, 57/58*, 627-632, 1996.

Gong, C. S., N. J. Cao, Y. Sun, and G. T. Tsao, "Production of L-Malic Acid from Fumaric Acid by Resting Cells of Brevibacterium sp.," *Applied Biochem. Biotechnology, 57/58*, 481-488, 1996.

Zheng, Y., H. M. Lin, J. Wen, N. Cao, X, Yu, C. S. Gong and G. T. Tsao, "Supercritical Carbon Dioxide Explosion as a Pretreatment for Cellulose Hydrolysis," *Biotechnology Letters,* (in press).

Srinivasan, N., N. Kasthurikrishnan, R. G. Cooks, M. S. Krishnan and G. T. Tsao, "On-line Monitoring with Feedback control of Bioreactors using Ethanol Tolerance Yeast by Membrane Introduction Mass Spectrometry," *Analytic Chimica Acta*., (in press).

Liu, D., S. Huang, M. Li, Y. Sun T. Liu F. Ouyang, G. T. Tsao, "Improvement of Productivity of Yeast Cell with a Novel Air-Lift Loop Reactor," *Applied Biochem. Biotechnology, 57/58*, 593-598, 1996.

Dominquez, J. M., C. S. Gong, and G. T. Tsao, "Pretreatment of Sugar cane Bagasse Hemicellulose Hydrolysate for Xylitol Production by Yeasts," *Applied Biochem. Biotechnology, 57/58,* 49-56, 1996.

Yang, X. and G. T. Tsao, "Enhanced Acetone-Butanol Fermentation Using Repeated Fed-Batch Operation Coupled with Cell Recycle by Membranes and Simultaneous Removal of Inhibitory Product Adsorption," *Biotechnology and Bioengineering, 47*, 444-450, 1995.

Lu, J., 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. Biotechnology, 51*, 29-41, 1995.

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. Biotechnology, 51,* 479-493, 1995.

Lu, Z., C. W. Yang, and G. T. Tsao, "Fermentation of Xylose to Glycerol by Rhizopus javanicus," *Applied Biochem. Biotechnology, 51*, 83-95, 1995.

Yang, C. W., Z. Lu, and G. T. Tsao, "Lactic Acid Production by Pellet-Form Rhizopus oryzae in a Submerged System," *Applied Biochem. Biotechnology, 51*, 57-71, 1995.

Venkat Venkatasubramanian

1988

Professor

Degrees

BTech, Chemical Engineering, University of Madras, India, 1977

MS, Physics, Vanderbilt University, 1979

PhD, Chemical Engineering, Cornell University, 1984

Interests

Process Fault Diagnosis and Supervisory Control

Process Hazards Analysis

Computer-Aided Molecular Design and Product Formulation

Synthesis of Operating Procedures for Batch Process Plants

Behavior of Complex Adaptive Systems

Intelligent Systems, Neural Networks, and Genetic Algorithms

Major Appointments

Editorial Board, *Process Safety Progress*

Member of the New Technology Task Force, American Institute of Chemical Engineers, 1996-97

Research Areas

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

DKit: A Hybrid Intelligent System for Real-time Fault Diagnosis of Complex Chemical Plants: Real-time process fault diagnosis deals with the timely detection and diagnosis of abnormal process conditions. Industrial statistics estimate the economic losses due to abnormal process situations to be about 20 billion dollars per year in the petrochemical industries alone in the U.S. Thus, fault diagnosis is a very important aspect of safe and optimal operation of chemical plants. For the past ten years, our research group has focused on this problem area, developing a variety of solutions using knowledge-based systems, neural networks, statistical techniques and analytical models.

As there is no single diagnostic approach that can successfully address all the complexities of industrial-scale diagnostic problems, a few years ago we embarked on the design of a hybrid, blackboard-based diagnostic environment, called DKit. DKit combines different diagnostic methods to perform collective problem solving, combining

the relative merits of the various approaches. The current version of DKit, implemented in G2, combines causal model-based diagnosis with a statistical classifier and a syntactic pattern recognition method. At present, our group is actively engaged in various research issues concerning the design and testing of DKit on real-time industrial data from a fluidized catalytic cracking unit (FCCU).

Due to the increasing importance of this problem area, Honeywell, a leading vendor of process control systems, recently formed the Abnormal Situation Management (ASM) Consortium, a technology-development partnership of leading oil companies and software vendors, to develop an intelligent system environment for operator support, called Abnormal Event Guidance and Information System (AEGIS). This four year, $16 million R&D project is funded to the extent of $8 million by the Advanced Technology Program (ATP) of the National Institute of Standards and Technology (NIST) of the Department of Commerce. The rest of the support comes from the consortium partners. Our group has been invited to be a part of this important and exciting research consortium to develop AEGIS. We are pleased that our contributions in the diagnosis area including DKit are being utilized in the design of next-generation process control systems through a close collaboration between LIPS researchers and the ASM personnel.

Automated Hazard and Operability Analysis: Process Hazards Analysis (PHA) is the systematic identification and mitigation of potential process hazards which could endanger the health and safety of humans and cause serious economic losses. This is an important activity in Process Safety Management (PSM) that requires a significant amount of time, effort, and specialized expertise. The importance of this activity is underscored by the Occupational Safety and Health Administration's (OSHA) PSM Standard Title 29 CFR 1910.119 which requires initial PHAs of all the processes covered by the standard to be completed by no later than May 26, 1997. Hazard and operability (HAZOP) analysis is the most widely used and recognized as a preferred PHA approach by the chemical process industries.

HAZOP analysis is the study of systematically identifying every conceivable deviation from the design intent, and all possible abnormal causes, and adverse hazardous consequences that can occur in a chemical plant. This is a difficult, labor- and knowledge-intensive, and time-consuming analysis. HAZOP analysis is typically performed by a group of experts poring over the process P&IDs for weeks. A typical HAZOP study can take 1-8 weeks to complete, costing about $10,000 per week. It is estimated that $2 billion will be spent collectively by the process industry between 1995-97, on PHA studies alone.

Given the enormous amounts of time, effort and money involved in HAZOP reviews, there exists considerable incentive to develop an automated approach to the HAZOP analysis of process plants. An automated system is needed that can reduce the time, effort and expense involved in a HAZOP review, make the review more thorough and detailed, minimize human errors and free the team to concentrate on the more complex aspects of the analysis which are difficult to automate. Towards that goal, an intelligent system called *HAZOPExpert* has been developed in the LIPS group.

The central ideas in *HAZOPExpert* are the separation of the knowledge required to perform HAZOP analysis into process-specific and process-general knowledge, and the use of generic HAZOP-digraph models for pro-

cess units. The process-specific knowledge consists of information about the materials used in the process, their properties (such as corrosivity, flammability, volatility, and toxicity) and the piping and instrumentation drawings (P&IDs) of the plant. The process-specific knowledge changes from plant to plant and is provided by the user. The process-general knowledge consists of the HAZOP-Digraph (HDG) models of the process units which are qualitative causal models developed specifically for hazard identification. These HDG models are the generic HAZOP models of the process units developed in an object-oriented and context-independent manner so that they can be used for a wide-variety of processes. The HAZOP inference engine contains the algorithms for finding abnormal causes, adverse consequences and for propagating process variable deviations. These methods allow for the appropriate interaction of the process-general and process-specific knowledge and identify only the abnormal causes and the adverse consequences which are realizable for a given process. The user interacts with the system through the graphical user interface (GUI), which consists of the P&IDs graphical editor and the graphical HDG model developer for knowledge acquisition and augmentation.

Currently research is in progress to develop this framework further to include batch process plants. We are also investigating a multiple-models approach which combines the qualitative digraph models with more precise dynamical models of process units for improved bounds on the predicted abnormal behavior. Efforts are also underway to include fault tree and reliability engineering models in the framework.

Computer-aided Molecular Design: The process of designing new molecules possessing desired physical, chemical and biological properties is an important endeavor in chemical, material and pharmaceutical industries. Industrial applications include designing composites and blends, drugs, agricultural chemicals such as pesticides or herbicides, refrigerants, solvents, paints and varnishes. With recent developments such as stricter penalties on environmentally unfriendly products and emphasis on value-added products and designer molecules, the search for novel materials has become an essential part of R&D in the above fields. The traditional approach for developing new materials is a lengthy and expensive trial-and-error procedure, usually involving the preliminary screening of hundreds, even thousands, of candidates. Hence, researchers have resorted to computer-aided molecular design (CAMD) approaches.

CAMD requires the solution of two problems: the *forward* problem, which predicts physical, chemical and biological properties from the molecular structure; and the *inverse* problem, which requires the identification of the appropriate molecular structure given the desired macroscopic properties. In this project, we have developed a CAMD framework that uses neural networks and genetic algorithms to address many of the difficulties in present CAMD approaches. Neural networks are networks of information processing elements that are very useful for nonlinear pattern recognition problems. Genetic algorithms are computer models of Darwinian concepts of evolution with natural selection. The neural network-based property prediction methodology develops nonlinear structure-property relationships for complex molecules, thus addressing the forward problem. The genetic algorithmic component tackles the inverse problem by proposing suitable candidates in an evolutionary manner, periodically subjecting the population to the survival of the fittest principle. This novel CAMD paradigm has been implemented in G2 and C++ as an interactive molecular design system called GENESYS. Current research involves parametric sensitivity analysis of the genetic algorithm for

large-scale CAMD, characterization of the search space and refinements to GENESYS. We are also applying GENESYS to real-life product design and formulation problems faced by the industrial sponsors of this project.

Systematic Synthesis of Operating Procedures for Batch Plants: Synthesis of operating procedures for batch plants involves the systematic generation of step by step instructions which an operator can implement to manage a batch plant safely and optimally. This is a labor- and knowledge-intensive task that often takes weeks of effort by experts to prepare a clear and error-free set of instructions even for a moderately complex plant. An automated system can reduce the time, effort and expense involved for this activity, make the procedures more thorough and detailed, and minimize human errors. Towards that goal, an intelligent system framework has been developed in this project.

The operating procedures are to be developed from information about the plant setup, process chemistry and recipe, and product requirements. The plant configuration information would consist of process equipment, their capabilities, constraints and their connectivities. The process chemistry and recipe information would comprise various steps, such as reaction and unit operations like filtration, centrifugation and drying, that were carried out in the laboratory in order to generate the desired product. The plant setup and process chemistry constitute process specific knowledge; that is, they give details about a particular process that has to be carried out in a certain plant. In addition, we have process general knowledge. These are models that tell us how to perform a certain type of operation in a particular kind of equipment.

The key issues towards solving the automation problem are knowledge representation and planning. The knowledge representation strategy should be able to handle both the process specific and process generic knowledge in a flexible manner that can facilitate easy modification, and also address the discrete event character of batch processes. We solve these needs by adopting object-oriented techniques to model process specific knowledge and a framework called Grafcets for representing the process generic knowledge. Grafcets is a discrete event modeling framework based on Petri nets concepts. Grafcets is ideal for representing task sequences that are encountered in batch plant operations.

Planning provides the control strategy that utilizes the process specific and process general knowledge to generate the exact sequence of tasks that need to be performed by the operator to produce the required product in a certain batch plant facility. We use hierarchical planning for the problem of sequence generation. This approach tackles the problem of sequencing the operations first at the level of operations like reaction and unit operations such as centrifugation and filtration. These can be called higher-level operations. Once the details of performing these operations are worked out, then the control strategy becomes more fine grained. It takes apart these higher-level operations and sequences the tasks that make up these operations. The nature of the planning strategy helps it exploit the structured modeling framework of Grafcets to come up with a feasible set of operating procedures.

Based on this framework, an intelligent system called iTOPS (Intelligent Tool for Operating Procedures Synthesis), has been implemented in Gensym's object-oriented expert system environment called G2. Current research involves testing and redesigning iTOPS on a large-scale industrial case study of a pharmaceutical process used by the industrial sponsor of this project.

Publications

Aoyama, A., F.J. Doyle and V. Venkatasubramanian, "Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control," *J. of Process Control*, 5 (6), pp. 375-386, 1995.

Aoyama, A., F.J. Doyle and V. Venkatasubramanian, "Control-Affine Neural Network Approach for Nonminimum-Phase Nonlinear Process Control," *J. of Process Control*, 6 (1), pp. 17-26, 1995.

Aoyama, A., F.J. Doyle and V. Venkatasubramanian, "Fuzzy Neural Networks for Nonlinear Process Control," *Engg. Applns. of Art. Intel.*, 8 (5), pp. 483-498, 1995.

Aoyama, A. and V. Venkatasubramanian, "Internal Model Control Framework Using Neural Networks for the Modeling and Control of a Bio-reactor," *Engg. Applns. of Art. Intel.*, 8 (6), pp. 689-701, 1995.

Vaidhyanathan, R. and V. Venkatasubramanian, "Digraph-based Models for Automated HAZOP Analysis," *J. of Rel. Engg. and Sys. Safety*, 50, pp. 33-49, 1995.

Venkatasubramanian, V., A. Sundaram, K. Chan and J. M. Caruthers, "Computer-Aided Molecular Design using Neural Networks and Genetic Algorithms," in *Genetic Algorithms in Molecular Modeling,* J. Devillers, (Ed.), Academic Press, 1996.

Vaidhyanathan, R., V. Venkatasubramanian and F. Dyke, "HAZOP Expert; An Expert System for Automating HAZOP Analysis," *Process Safety Progress*, 15(2), 1996.

Srinivasan, R. and V. Venkatasubramanian, "Petri Net-Digraph models for automating HAZOP analysis of batch process plants," in Proceedings of the *European Symposium on Computer-Aided Process Engineering 6*, Rhodes, Greece, May 1996.

Shin, D. and V. Venkatasubramanian, "Intelligent Tutoring System Framework for Operator Training for Diagnostic Problem Solving," in Proceedings of the *European Symposium on Computer-Aided Process Engineering 6,* Rhodes, Greece, May 1996.

Vaidyanathan, R. and V. Venkatasubramanian, "Experience with an Expert System for Automated HAZOP Analysis," in Proceedings of the *European Symposium on Computer-Aided Process Engineering 6*, Rhodes, Greece, May 1996.

Meeting Presentations

Vaidhyanathan, R. and V. Venkatasubramanian, "Digraph-based Models for Automating the HAZOP Analysis of Chemical Plants," AIChE Annual Meeting, Miami, FL, November 1995.

Mylaraswamy, D., A. Wallen, V. Venkatasubramanian and K-E. Arzen, "A Model-based Hybrid Neural Network Architecture for Fault Diagnosis," AIChE Annual Meeting, Miami, FL, November 1995.

Srinivasan, R. and V. Venkatasubramanian, "Integrating Petri Nets and Digraphs to represent the HAZOP Knowledge of Batch Processes," AIChE Annual Meeting, Miami, FL, November 1995.

Aoyama, A., V. Venkatasubramanian and F.J. Doyle, "Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control," AIChE Annual Meeting, Miami, FL, November 1995.

Rengaswamy, R., T. Hagglund and V. Venkatasubramanian, "A Qualitative Shape Analysis Procedure for Automatic Monitoring of Control Loop Performance," AIChE Annual Meeting, Miami, FL, November 1995.

Doyle, F.J., T. Kendi and V. Venkatasubramanian, "Purdue Control Modules: A MATLAB Package for Undergraduate Process Control," AIChE Annual Meeting, Miami, FL, November 1995.

Venkatasubramanian, V., "Intelligent Systems for Process Diagnosis and Safety," *CHEMCON'95*, Madras, India, December 1995.

Invited Lectures

HAZOPExpert: An Intelligent System for Automating Process Hazards Analysis, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, July 1995.

A Model-based Framework for Automated Process Hazards Analysis, Department of Chemical Engineering, Loughborough Institute of Technology, Loughborough, U.K., July 1995.

Application of Intelligent Systems in Process Diagnosis, Safety and Design, Imperial Chemical Industries, Runcorn, U.K., July 1995.

"A Perspective on Intelligent Systems for Process Hazards Analysis," International Conference on *Intelligent Systems in Process Engineering (ISPE'95),* Snowmass, CO, July 1995.

Computer-Aided Operating Procedure Synthesis for Batch Process Plants, G. D. Searle and Co., Skokie, IL, September 1995.

DKit: A Hybrid Intelligent System for Real-time Fault Diagnosis of Complex Chemical Plants, Exxon R&D, Florham Park, NJ, September 1995.

HAZOPExpert: An Intelligent System for Automating Process Hazards Analysis, Gensym Corporation, Cambridge, MA, October 1995.

Computer-Aided Molecular Design Using Neural Networks and Genetic Algorithms, Indian Institute of Technology, Madras, India, December 1995.

AI Applications in Process Fault Diagnosis and Safety, Anna University, Madras, India, January 1996.

AI Approaches to Computer-aided Molecular Design, The Lubrizol Corporation, Cleveland, OH, February 1996.

HAZOPExpert: An Intelligent System for Automating Process Hazards Analysis, Department of Chemical Engineering, University of Edinburgh, Edinburgh, Scotland, March 1996.

Chaired Conferences/ Symposia

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

Chairman, *Computer Integrated Manufacturing in Process Industries* Session, AIChE Annual Meeting, Miami, FL, November 1995.

Area Coordinator, *Computer Applications in Chemical Engineering* (8 sessions), ASEE Summer School in Chemical Engineering, August 10-15,1997, Snowbird, UT.

Member, International Program Committee, *Seventh European Symposium on Computer-Aided Process Engineering,* ESCAPE 7, Trondheim, Norway, May 1997.

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

Environmental Applications of Separation Techniques

Adsorption of Chemicals and Biochemicals

Mass Transfer in Chemical and Biological Systems

Multicomponent Ion Exchange and Adsorption in Large Scale Chromatography and Continuous Chromatography

Awards and Major Appointments

NSF Faculty Award for Women Scientists and Engineers, 1991-1996

Member of NIH Study Section of Surgery and Bioengineering, 1992-1996

Research Areas

Ion Exchange Processes for Removing Cesium from Nuclear Waste Solutions: Over the last fifty years, more than 100 million gallons of radioactive wastes generated mostly from the production of nuclear weapons have been stored in over 300 underground single-shell or double-shell tanks at Hanford, Savannah River, Oak Ridge, and other DOE facilities. It is estimated that about half of the single shell tanks are leaking, posing serious environmental threats to many states. Efficient separation technologies are needed to treat the wastes and to allow safe long-term storage of the separated wastes. Remediation of the tank waste is estimated to cost over 100 billion dollars. This is considered by many experts one of the greatest technical and financial challenges facing the U.S. today.

Major contributors to the radioactivity in the wastes are cesium and strontium. The removal of cesium, from the supernatants is an important early step in the waste treatment process. We are collaborating with researchers from Westinghouse and Oak Ridge National Laboratories in developing an ion exchange process for the remediation. The challenge is to develop highly selective and efficient continuous processes for removing low (1-1000 mM) concentrations of radioactive Cs^+ ions from concentrted aqueous solutions (1-14 M) of sodium hydroxide, sodium nitrite, and other electrolytes. We have devleoped realistic models for correlating multicomponent ion exchange equilibrium data.

We have also developed detailed dynamic models of fixed-bed ion exchange, accounting for competitive ion exchange equilibria and mass transfer effects. Detailed process simulations are used to explore innovative designs of carousel processes. We hope these processes will be used in the future for efficient large scale continuous waste processing.

Removal and Recovery of Organics from Water and Wastewaters: Contamination of water supplies by synthetic organics, pesticides, herbicides, and other industrial chemicals is a widespread problem in the U.S. and many other countries. Many of the chemicals are known to be carcinogenic and must be removed to safeguard drinking water supplies and the environment. Among many treatment techniques, adsorption using activated carbon beds has been the best available technology for removing dissolved organics from a dilute (ppm level) solution. Because of high selectivity, activated carbon beds can achieve virtually complete removal of many organics. This technique, however, is quite expensive. Cost of treatment ranges from $0.1 to $19.00 per 1000 gal. This high cost is due to (1) process inefficiency as a result of low throughput and low capacity utilization, (2) high capital and labor costs due to the nature of batch operation in conventional technologies, (3) sorbent attrition and incomplete, costly regeneration, and (4) loss of the organics during sorbent regeneration. Research in our laboratory aims to find solutions to these key issues. Our long-term research objectives are to advance the fundamental knowledge in adsorption and to develop efficient and economical continuous adsorption technologies to reduce water pollution and to recover organics and other chemicals from wastewaters.

Isolation and Purification of Taxol from Plant Tissue Culture Broth and Needle Extract: Taxol, a promising anti-cancer agent, was first found in extracts from the bark of the Pacific yew tree. Because of increasing demand for taxol and limited availability of the bark, many studies have been devoted to finding alternative sources. Plant tissue culture and *Taxus* natural plant tissues are among the most promising alternatives. We have developed a low pressure liquid chromatography process for the separation of taxol directly from plant tissue culture broth. In addition, a separation process which consists of extraction, low pressure liquid chromatography, and preparative HPLC has also been developed for the isolation and purification of taxol from *Taxus* needles. Our current processes can achieve high recovery (90%) and high purity (~95%) at an estimated recovery and purification cost of less than $100/g. Ongoing research aims to improve the purity level and to further reduce the recovery and purification cost.

Publications

Clark, W.R., W. L. Macias, B.A. Molitoris, and N.-H.L. Wang, "Plasma Protein Adsorption to Highly Permeable Hemodialysis Membranes," *Kidney International*, *48,* 481-488, 1995.

Koh, J.-H., N.-H.L. Wang, and P.C. Wankat, "Ion Exchange of Phenylalanine in Fluidized/Expanded Beds," *Ind. Eng. Chem. Res., 34*, 2700-2711, 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, 11*, 3177 - 3183, 1995.

Ma, Z., R.D. Whitley, and N.-H. L. Wang, "Pore and Surface Diffusion in Multicomponent Adsorption and Liquid Chromatography Systems," *AIChE J,* 42 (5) 1244-1262, 1996.

Ma, Z., D. Tanzil, B.W. Au and N.-H.L. Wang, "Estimation of Solvent Modulated Linear Adsorption Parameters of Taxanes from Dilute Plant Tissue Culture Broth," *Biotech. Progresss*, in press.

Wu, D.J., Z. Ma, B. Au and N.-H.L. Wang, "Recovery of Paclitaxel from Plant Tissue Culture Broth Using Low Pressure Liquid Chromatography," *AIChE J.*, 1996, in press.

Ernest, M.V. Jr., R.D. Whitley, Z. Ma and N-H.L. Wang, "Effects of Mass Action Equilibrium on Fixed-Bed Multicomponent Ion Exchange Dynamics," *IEC Research*, 1996, accepted.

Meeting Presentations

Symposium on Ion Exchange in Metal Ion and Molecular Separations, M. Ernst, Jr., R.D. Whitley, Z. Ma, and N.-H.L. Wang, "Effects of Mass Action Equilibrium and Intraparticle Diffusion in Fixed-Bed Multicomponent Ion Exchange Systems," AIChE Annual Meeting, Miami Beach, FL, November 12-17, 1995.

Symposium on Bioseparation and Ion Exchange, K. Khan, S. Patel, Z. Ma, and N.-H.L. Wang, "Biomolecule Adsorption in Affinity Chromatography," AIChE Annual Meeting, Miami Beach, FL, November 12-17, 1995.

Invited Lectures

Invited lecture on "Applications of Ion Exchange and Adsorption for Wastewater Treatment," Oak Ridge National Laboratory, Oak Ridge, TN, July 11, 1995.

Invited talk on "Parallel Pore and Surface Diffusion Large-Scale Liquid Chromatography Systems," in the Symposium on Multiphase Flow, Microstructured Media, Diffusion, and Biological Transport, The 26th Annual Meeting of the Fine Particle Society, Chicago, IL, August 22-25, 1995.

Invited seminar on "VERSE-Evolution from Fixed Beds to Simulated Moving Beds," U.S. Filters, Rockville, IL, September 26, 1995.

Invited seminar on "VERSE-Evolution from Fixed Beds to Simuated Moving Beds," Reliance Chemicals, Chicago, IL, September 12, 1995.

Invited seminar on "Liquid Chromatography," Dow Corning, Midland, MI, May 9, 1996.

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

Teaching Improvement

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. Unusual pressure effects have been observed and analyzed. Vacuum, pressure, steam and thermal swing regeneration methods are being explored.

Other separations research in progress: 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. Combined adsorption and reaction is being analyzed.

Awards and Major Appointments

Appointed Associate Editor of *Chemical Engineering Education*

Publications

Koh, J.-H., N.-H.L. Wang, and P.C. Wankat, "Ion-Exchange of Phenylalamine in Fluidized / Expanded Beds," *Ind. Engr. Chem. Research*, 34, 2700-2711, 1995.

Simms, C., Arumugam, B., and P.C. Wankat, "Modified Displacement Chromatography Cycles for Gas Systems," *Chem. Engr. Sci.*, 51, 701-711, 1996.

Wankat, P.C and K.S. Knaebel, "Mass Transfer," Section 5B in Perry's *Handbook of Chemical Engineering,* 7th ed., Green, D. (Ed.), McGraw-Hill, New York, (in press).

Arumugam, B.K. and P.C. Wankat, "Pressure Behavior During the Loading of Adsorption Systems," Proceedings Fifth International Conference on Adsorption, (in press).

Editorial Boards

Separation and Purification Methods, Editor-in-Chief

Chemical Engineering Education, Associate Editor

Separation Science and Technology

Adsorption

Invited Lectures

"Improving Lectures," Mechanical Engineering, M.I.T., February 9, 1996; Chemical Engineering, University of South Carolina, April 18, 1996.

"The Efficient Professor," Seventh National Conference on College Teaching and Learning, Jacksonville FL, March 22, 1996.

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
$440,389	**R.P. Andres** Army Research Office Electronic Conduction in Molecular Nanostructures	07/92-06/97
$366,426	**R.P. Andres** **R. Reifenberger** National Science Foundation Synthesis of Nanometer Diameter Particles and Measurement of Particle-Particle and Particle Substrate Interactions	05/92-07/97
$65,396	**R.P. Andres** Arco Chemical Co. Development of Selective Catalyst for Proplyene Epoxidation	05/95-05/97
$10,000	**O.A. Basaran** Exxon Education Foundation Research into Micron-and Sub-Micron Size Particles	10/94-09/96
$10,000	**O.A. Basaran** Dow Corning Corporation Computational Analysis of Fluid Mechanics of Distillation Trays	01/96-12/99
$70,000	**O.A. Basaran** NASA Forced Oxcillations of Pendant and Sessile Drops	06/96-06/97
$62,718	**J.M. Caruthers** AFOSR Fundamental Models for Predicting Lifetime Performance of High Performance Polymeric Materials	03/95-03/97
$21,240	**J.M. Caruthers** Purdue Research Foundation Phase Equilibria of Polymer Mixtures	03/95-97
$11,992	**J.M. Caruthers** Class of 1941 Teaching Innovation Grant Development of Computer Simulation Modules for Teaching	05/95-99/99
$45,000	**W.N. Delgass** Dupont Central Research & Development Research for Expanding the Horizons and Overall Understanding of Heterogeneous Catalysis	12/94-99/99

Award Amount	PI/Sponsor/Title	Project Period
$22,000	**W.N. Delgass** Trask Trust Fund Support for Exploratory Research	09/94-02/96
$11,040	**W.N. Delgass** Purdue Research Foundation Dehydration of 2,3 Butanedial to Methyl Ethyl Ketone over Zeolite Catalysis	04/96-04/97
$275,000	**F.J. Doyle** National Science Foundation NSF/NYI Matching Funds	03/94-99/99
$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	06/94-03/96
$21,240	**F.J. Doyle** Purdue Research Foundation Specialized Mathematical Programming Methods in the Model Predictive Control of Large Scale Systems	04/95-05/97
$78,500	**F.J. Doyle** Office of Naval Research Neurobiologically Inspired Approaches to Nonlinear Process Control & Modeling	05/96-10/96
$242,425	**E.I. Franses** National Science Foundation Adsorption Dynamics of Mixed Surfactants and Proteins at Air/Water Interfaces: Applications to Foams and Lung Surfactant	08/93-01/97
$11,040	**E.I. Franses** Purdue Research Foundation Effect of Processing Method on the Quality, Stability and Transport Properties of Thin Organic Films	04/96-04/97
$5,000	**E.I. Franses** Johnson, S.C. & Son Inc. Unrestricted Research Support	03/96-03/97
$ 50,881	**R.A. Greenkorn** Indiana Dept. of Enviromental Management Indiana Pollution Prevention Institute	06/93-06/97

Award Amount	PI/Sponsor/Title	Project Period
$42,874	**R.A. Greenkorn** Showalter Trust The Movement of Pollutants Underground	06/94-06/96
$11,040	**R.A. Greenkorn** Purdue Research Foundation NMR Imaging of Mixing During Flow in Heterogeneous Porous Media	07/96-07/97
$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
$300,000	**H.S. Lackritz** National Science Foundation NSF Presidential Faculty Fellows Program	08/93-02/97
$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
$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
$3,000	**H.S. Lackritz** National Science Foundation Polymeric Thin Films for Photonic Applications	08/96-02/97
$312,500	**J.F. Pekny** National Science Foundation/Industry Presidential Young Investigator Award	08/90-09/95
$240,501	**J.F. Pekny** **G.V. Reklaitis** NSF A Comprehensive Approach to Chemical Process Scheduling Problems	04/94-08/97
$69,570	**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	10/94-10/96
$10,200	**N.A. Peppas** International Association for Pharmaceutical Tech. European Journal of Pharmaceutics and Biopharmaceutics	10/93-99/99

Award Amount	PI/Sponsor/Title	Project Period
$214,218	**N.A. Peppas** National Science Foundation Polymer Dissolution	09/92-08/96
$189,820	**N.A. Peppas** National Science Foundation Multifunctional Polymerization Kinetics and Network Structure Thereof	08/93-01/97
$10,972	**N.A. Peppas** NATO (N. Atlantic Treaty Organization) Investigation of Water and Solute Diffusion in Hydrophilic Polymers	03/94-01/98
$60,000	**N.A. Peppas** Showalter Trust Showalter Distinguished Professorship in Biomedical Engineering	11/93-06/97
$221,212	**N.A. Peppas** PHS-NIH PH Sensitive Complex Hydrogels and IPNS for Drug Release	09/95-09/96
$3,187	**N.A. Peppas** Nagai Foundation Foreign Travel for Research	06/96-06/97
$10,200	**N.A. Peppas** Purdue Research Foundation Glucose-Sensitive Systems for Insulin Delivery	01/96-01/97
$50,000	**N.A. Peppas** Showalter Trust Novel Mucoadhesive Biopolymers for the Targeted Delivery of Peptides and other Drugs to Tissue	07/96-07/97
$45,000	**D. Ramkrishna** American Institute of Chemical Engineers Investigation of Shelf-Life of Food Emulsions	05/92-04/97
$90,000	**D. Ramkrishna** Office of Naval Research Modelling of Microbiological Remediation of Shipboard Waste Effluents	04/94-09/96
$230,084	**G.V. Reklaitis** Shell Companies Foundation, Inc. Shell Oil Company Foundation Fellowship	09/85-08/96
$155,600	**G.V. Reklaitis** E.I. du Pont de Nemours & Company E.I. du Pont de Nemours & Company Fellowhsip	09/81-08/96

Award Amount	PI/Sponsor/Title	Project Period
$1,856,143	**G.V. Reklaitis** U.S. Department of Education Purdue Program for Graduate Assistance in Chemical Engineering Areas of National Need	09/92-08/96
$85,561	**G.V. Reklaitis** C.D. McAllister Endowment Goddard Fellowship	06/90-99/99
$118,250	**G.V. Reklaitis** National Consortium Graduate Minorities Engineering & Science National Consortium for Minorities Fellowship	09/92-12/96
$67,823	**G.V. Reklaitis** Oak Ridge Associated Universities Computational Science Graduate Fellowship Program	09/92-08/96
$350,000 +250,000 (in kind)	**F.J. Doyle** **J.F. Pekny** **G.V. Reklaitis** **V. Venkatasubramanian** Computer Integrated Process Operations Center Individually Supported	05/96-99/99
$150,000	**G.V. Reklaitis** **R.G. Squires** Procter & Gamble Company Procter & Gamble Chemical Engineering Education Module	07/93-06/96
$135,000	**G.V. Reklaitis** USDA Developing Environmentally and Economically Sustainable Food Processing Systems	09/95-09/97
$14,000	**G.V. Reklaitis** National Science Foundation Travel Grant for U.S. Academic Participants in Workshop on World-Wide Ind-Aca.-Govt. Research Collaboration Models in the Chemical Sciences and Engineering	01/96-01/97
$151,100	**E.M. Sevick-Muraca** National Science Foundation National Young Investigator Biomedical Optical Imaging	09/94-09/97
$507,162	**E.M. Sevick-Muraca** Public Health Service N.H. Frequency-Domain Photon Migration Imaging for Breast Cancer Screening	08/94-05/97

Award Amount	PI/Sponsor/Title	Project Period
$133,491	**E.M. Sevick-Muraca** Mallinckrodt Medical Contrast Agents for Biomedical Optical Imaging	08/94-09/96
$42,728	**E.M. Sevick-Muraca** University of Tennessee Process Monitoring with Measurement of Photon Migration	09/94-08/96
$143,070	**E.M. Sevick-Muraca** PHS-NIH National Cancer Institute Photon Migration Measurements for Tissue Diagnostics	07/95-07/97
$35,000	**E.M. Sevick-Muraca** E.I. duPont de Nemours & Co. Process Measurement	09/95-99/99
$81,660	**R.G. Squires** National Science Foundation Educational Applications of Computer Simulations of Chemical Engineering Processes	02/94-01/97
$295,940	**C.G. Takoudis** **C. Neudeck** **E. Kvam** National Science Foundation REU Site for Microelectronic Materials and Processing	05/92-10/96
$415,000	**C.G. Takoudis** **M.J. Weaver** National Science Foundation Raman Spectroscopic Characterization of Transition-Metal Surfaces in Catalytic Reactor Systems	09/93-02/97
$83,981	**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	10/92-09/96
$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	07/93-06/97
$530,891	**V. Venkatasubramanian** PHS-CDC National Institute of Occupation, Safety and Health A Knowledge-Based Framework to Automate Hazop Analysis	09/93-09/96
$20,400	**V. Venkatasubramanian** Purdue Research Foundation Computer-Aided Molecular Design Using Genetic Algorithms	11/94-11/96
$10,000	**V. Venkatasubramanian** Honeywell, Inc. A. Hybrid Intelligent System for Real-Time Process Fault Diagnosis	12/95-09/96
$56,000	**V. Venkatasubramanian** Lubrizol Corporation A. Proposal to Develop a Neural Network - Genetic Algorithm Framework for Product Design and Formulation	12/95-12/96
$300,000	**V. Venkatasubramanian** National Science Foundation Process Systems Tools for the Development and Management of Environmentally and Economically Conscious Mfg.	09/95-08/98
$250,000	**N.-H.L. Wang** National Science Foundation NSF Faculty Awards for Women Scientists and Engineers	11/91-10/96
$17,000	**N.-H.L. Wang** Trask Trust Fund Beta-Site Testing and Further Development of Verse	01/93-07/97
$103,305	**N.-H.L. Wang** Bristol-Myers Squibb Co. Development of a Continuous Adsorption Process to Recover and Purify Paclitaxel from Plant Tissue Culture Broth	12/95-11/96
$10,200	**N.-H.L. Wang** Purdue Research Foundation Design a New Adsorption Process for Removal of Organics from Water and Wastewater	01/96-01/97

Award Amount	PI/Sponsor/Title	Project Period
$50,000	**N.-H.L. Wang** Showalter Trust Removal of Toxic Organics from Water and Wastewater	07/95-07/97
$211,449	**P.C. Wankat** National Science Foundation Multicomponent Adsorption Processes	05/94-04/97
$10,200	**P.C. Wankat** Purdue Research Foundation Development of Simultaneous Fermentation/Separation from Lactic Acid Production	09/95-09/96

Thesis Projects

Graduate Student *Major Professor*	**Thesis** **Title**	**Degree** **Date Granted**
Bereolos, Peter J. *Chao & Talbot*	Molecular Simulation of Phase Equilibria and Transport Properties	PhD
Fu, Chu-Yun Stacey *Lackritz*	Polymer Physics and Structural Property Relationships of Thermally Stable Polyarylene Ethers for Second Order Nonlinear Optics	PhD August 4, 1995
Kar, Kevin Brian *Wiest*	Nonisothermal Shear Flow of Polymer Melts	MS August 4, 1995
Liu, Lee-Yin *Lackritz*	Electric Field Effects and Molecular Motion in Polymer Thin Films for Second Order Nonlinear Optical Applications	PhD August 4, 1995
Rengasamy, Raghunathan *Venkatasubramanian*	A Framework for Integrating Process Monitoring, Diagnosis, and Supervisory Control	PhD August 4, 1995
Starry, Adam Ben *Caruthers*	An Investigation of Spatially Heterogeneous Mobility Domains for Liquids in the Glass Transition Region	PhD August 4, 1995
Sullivan, Leah Ann *Lackritz*	Dynamic Mechanical Analysis and Dielectric Relaxation for Second Order Nonlinear Optical Applications	MS August 4, 1995
Sy Siong Kiao, Rogelio *Caruthers & Chao*	Models for the Prediction of the Pressure-Volume-Temperature Relationship and the Diffusion Coefficient in Polymer Melts	PhD August 4, 1995
Yang, Chien-Wen *Tsao*	Lactic Acid Production by Rhizopus oryzae in Submerged Systems	PhD August 4, 1995
Achanta, Srinivas *Okos, Kessler, Cushman*	Moisture Transport in Shrinking Gels During Drying	PhD December 16, 1995
Adams II, Robert C. *Delgass*	Zeolite Encapsulated Vanadium Oxo Species for the Selective Catalytic Reduction of Nitric Oxide by Ammonia	PhD December 16, 1995
Buccilli, Sergio *Okos, Kessler, Maier*	Starch Gelatinization and Moisture Transport in Corn Kernels During Cooking	MS December 16, 1995

Graduate Student *Major Professor*	**Thesis** **Title**	**Degree** **Date Granted**
Honkomp, Steven J. *Reklaitis & Venkatasubramanian*	Development of a Model Based Testing Framework for Reactive Scheduling Under Uncertainty	MS December 16, 1995
Hsieh, Hsing-Chun Julia *Takoudis*	Fundamental Studies of Hydrogen Passivated Silicon (100) Surfaces	MS December 16, 1995
Irwin, Nancy C. *Greenkorn*	Experimental Investigation of Scale-Dependent Dispersion in Laboratory-Scale Heterogeneous Porous Media	MS December 16, 1995
Koh, Joon-Ho *Wankat & Wang*	Ion-Exchange in Fluidized / Expanded Beds for Recovery of L-Phenylalanine	PhD December 16, 1995
Mahoney, William J. *Andres*	Synthesis of Nanoscale Clusters Using Atmospheric Arc Evaporation and Measurement of Cluster-Substrate Interactions	PhD December 16, 1995
McWilliams, Douglas S. *Caruthers*	The Effect of Thermal History on the Structural Relaxation and Thermovisco-elasticity of AmorphousPolymers	PhD December 16, 1995
Peters, Esly A. *Lackritz*	Temperature, Chromophore and Electric Field Effects in Contact Poled Polymer Thin Films Using Second Harmonic Generation and Dielectric Technique	MS December 16, 1995
Ramakrishnan, Ramasubramanian *Pekny*	A Mathematical Programming Approach for Lattice Molecular Simulations	PhD December 16, 1995
Stack, Alexander *Doyle*	The Optimal Control Structure: A Measure for Control-Relevant Nonlinearity	MS December 16, 1995
Vaidhyanathan, Ramesh *Venkatasubramanian*	A Model-Based Framework for Automating HAZOP Analysis of Continuous Process Plants	PhD December 16, 1995
Wang, Jinlin *Caruthers*	Predictions of Nonlinear Thermoviscoelastic Properties of Amorphous Polymers	PhD December 16, 1995
Buss, Michael R. *Andres*	Gas Aggregation Synthesis of Nanometer Diameter Magnetic Clusters	MS May 4, 1996

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Chen, Shannon *Takoudis*	Fundamental Studies on Yield and Growth Rate During Low Temperature Silicon Selective Epitaxial Growth in a Reduced-Pressure Pancake Reactor	MS May 4, 1996
Cho, Daechul *Franses & Narsimhan*	Dynamics of Protein Adsorption at Air-Water Interfaces	PhD May 4, 1996
Heemstra, Douglas George *Doyle*	Practical Nonlinear Model Identification and Control Implementaion	MS May 4, 1996
Krishnaswami, Soundararajan *Ramkrishna & Caruthers*	Stochastic Modelling and Simulation of Polymer Conformation in External Fields	PhD May 4, 1996
Ramakrishna, Ramprasad *Ramkrishna*	Cybernetic Modeling of Microbial Growth on Substitutable Substrates. Applications in Bioremediation	PhD May 4, 1996
Scott, Robert Allan *Peppas*	An Experimental Study of Acrylic Acid Solution Polymerizations	MS May 4, 1996
Subrahmanyam, Sriram *Pekny & Reklaitis*	Issues in Design and Planning of Batch Chemical Plants	PhD May 4, 1996
Trinh, Sinh Han *Ramkrishna*	Pattern Formation in Catalytic Packed Bed Reactors	PhD May 4, 1996
Wright, Shelia *Peppas*	Size Exclusion Phenomena in Drug Transport	MS May 4, 1996

Course Offerings and Seminars 1995-1996

Course Offering - Fall 1995

Class	Course Title	Instructor	Enrollment
201,301,401	Co-op Seminar	Squires	134
205	Chem. Engr. Calculations	Kessler	111
211	Chem. Engr Thermodynamics	Greenkorn	82
306	Design of Staged Separation	Wang	132
320	Statistical Modeling & Quality En.	Venkatasubramanian	103
348	Chem. Reaction Engineering	Takoudis	72
377	Momentum Transfer	Andersen	148
378	Heat and Mass Transfer	Houze	91
434	Chem. Engr. Laboratory I	Muench, Eckert Franses, Talbot	159
456	Process Dyanmics & Control	Doyle	188
461	Biomedical Engineering	Hannemann	42
496	Chem. Engr. Honors Lab	Delgass	14
540	Transport Phenomena	Sevick-Muraca	24
544	Structure and Prop. of Poly. Mat.	Peppas	45
597B	Chem. Process Industry	Hannemann	76
597H	Chem. Engineering Honors	Peppas	21
597O	Comp. Intgd. Proc. Opertn.	Doyle	32
597T	Biochemical Engineering	Ladisch	82
610	Advanced Chem. Engr. Thermo	Talbot	26
620	Transport Phenomena I	Caruthers	23
630	Applied Math. for Chem. Engr.	Pekny	21
632	Linear Operator CHE	Ramkrishna	5
697K	Advanced Kinetics	Andres	9
697Y	Mech, Elct, Opt Prop Ply	Lackritz	7

Special Projects:

411	Chem. Engr. Science. Research Projects	30
412	Chem. Engr. Design. Research Projects	14
498	Research in Chemical Engineering I	16

Course Offering - Spring 1996

Class	Course Title	Instructor	Enrollment
201,301	Co-op Seminar	Squires	87
205	Chem. Engr. Calculations	Andres	64
211	Intro. to Chem. Engr Thermo.	Squires	106
320	Statistical Modeling & Qual. Enhan.	Eckert	123
348	Chem. Reaction Engineering	Doyle	167
377	Momentum Transfer	Houze	61
378	Heat and Mass Transfer	Kessler	136
430	Principles of Molecular Engr.	Lackritz	192
435	Chem. Engr. Laboratory I	Muench, Eckert Franses, Lackritz, Bell, Squires	172
442	Chemistry and Engr. of High Poly.	Bell	73
450	Design & Analyis of Proc. Systems	Reklaitis	187
510	Intro to Chemical Engr. Thermo	Talbot	18
577	Flow Phen Porous Media	Greenkorn	8
597C	Polymer Science Engr. Lab.	Caruthers	4
597M	Adv. Chem E. Measmnt Lab	Delgass	3
597V	Artificial Intelligence	Venkatasubramanian	17
621	Transport Phenomena II	Ramkrishna	16
623	Separation Processes	Wang	13
660	Chemical Reaction Engineering	Takoudis	21
697B	Finite Element Anly Che	Basaran	14
697M	Biomedical Phenomena	Peppas	14

Special Projects:

411	Chem. Engr. Science Research Project	21
412	Chem. Engr. Design Research Project	13
499	Research in Chemical Engineering II	16

Seminars - Fall 1995

Speaker	Title	Date
Mr. Eugene R. Allspach Group Vice President Manufacturing & Manufacturing Services USI Division Quantum Chemical Corporation 11500 Northlake Drive Cincinnati, OH 45249	Non-Technical Skills for Successful Technical Careers	September 21, 1995
Professor Paul Barton Chemical Engineering Department Massachusetts Institute of Technology Cambridge, MA 02139-4307	Synthesis and Analysis of Batch Processes with Integrated Solvent Recovery and Recycling	October 5, 1995
Professor Wei-Shou Hu Chemical Engineering & Material Science Department University of Minnesota Minneapolis, MN 55455	Metabolic Fluxes in Mammalian Cell Systems and Bioartificial Liver	October 12, 1995
Professor Britton Chance Department of Biochemistry & Biophysics D501 Richards Building School of Medicine University of Pennsylvania Philadelphia, PA 19104-6089	Highly Sensitive Object Location in Highly Scattering Media: Breast Tumors and Brain Bleeds	October 19, 1995
Dr. Greg McKenna Polymers Division National Institute of Standards and Technology Gaithersburg, Maryland 20899	Physical Aging and its Implications for the Long Term Performance of Polymers and Composites	October 26, 1995
Dr. Mark Kramer Gensym Corporation 125 Cambridge Park Drive Cambridge, MA 02140	What's Happened to Artificial Intelligence	November 2, 1995

Seminars - Fall 1995 (continued)

Speaker	Title	Date
Dr. George Coustron E.I. duPont de Nemours & Co. Experimental Station Building 262 Wilmington, DE 19880	Toward Understanding VPO - Combining Material Science with Reaction Engineering	November 30, 1995
Prof. Larry V. McIntire Chemical Engineering Department Rice University Houston, TX 77251	Flow Modulation of Molecular Specificity and Leucocyte Endothelial Cell Adhesion	December 7, 1995

Seminars - Spring 1996

Speaker	Title	Date
Professor T. Alan Hatton Chemical Engineering Department Massachusetts Institute of Technology Cambridge, MA 02139-4307	Polymeric Solvents for Minimizing Pollutants in the Pharmaceutical Industries	February 15, 1996
Professor Julia M. Ross Dept. of Chemical & Biochemical Engineering University of Maryland Baltimore, MD 21228	The Pathogenesis of Infection: Molecular Mechanisms of Bacterial Adhesion to Collagen under Dynamic Shear Conditions	February 22, 1996
Dr. Gustavo Larsen Dept. of Chemical Engineering University of Nebraska Lincoln, NE 68588-0126	Catalytic Properties and Characterization of Strong Solid Acids	February 29, 1996
Dr. John Sherman UOP 50 East Algonquin Road Des Plaines, IL 60017-5016	Zeolites for Adsorptive Separations	March 21, 1996
Professor Rutherford Aris Chemical Engineering and Materials Science Dept. University of Minnesota Minneapolis, MN 55455	Reflections on Keats' Equations	March 28, 1996
Prof. James B. Rawlings Chemical Engineering Department University of Wisconsin-Madison Madison, WI 53706-1691	Modelling Dynamics and Control of Particulate Reactors	April 2, 1996
Professor John H. Seinfeld Chemical Engineering Dept. California Institute of Technology Pasadena, CA 91125	Aerosols: The Gremlin in The Greenhouse	April 11-12, 1996 Kelly Lecturer
Dr. Frank Allgower Institut fur Systemdynamik und Regelungstechnik Universitat Stuttgart Germany	Nonlinear Process Control — Just a Theoretical Discipline —	April 25, 1996
Dr. Mohsen A. Khalili DuPont Research and Engineering Wilmington, DE	The Role of Particle Size Distribution Measurement Laboratory in Industry	May 2, 1996