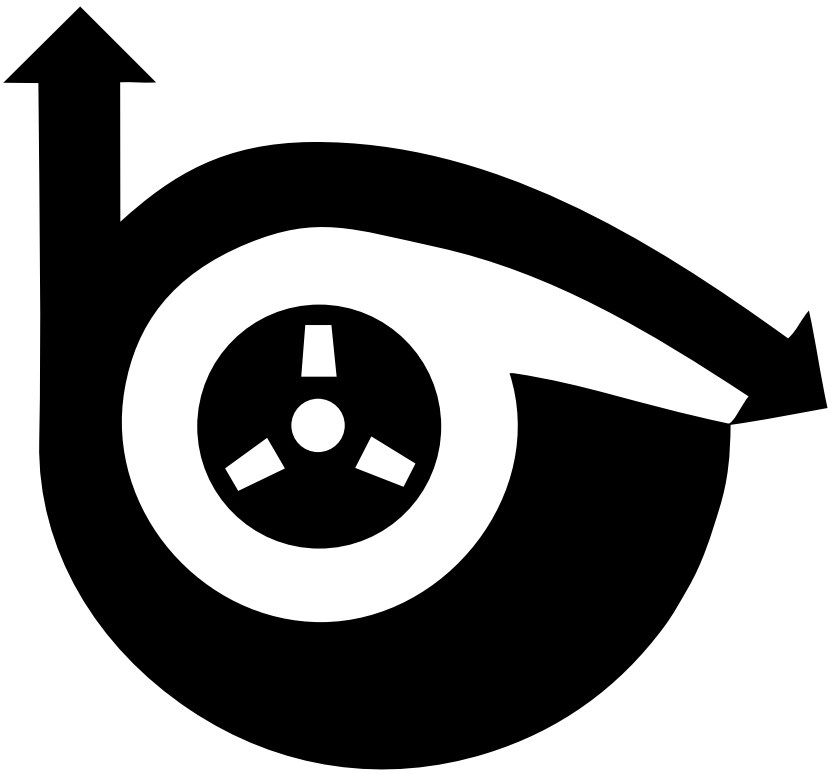
The School of Chemical Engineering

Annual Report

July 1, 1997-June 30, 1998



Purdue University

West Lafayette, Indiana

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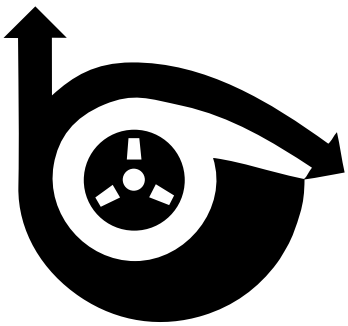


1997-1998

Academic Year Highlights

The School of Chemical Engineering

Faculty Affairs

Faculty Appointments

In January 1998, Dr. Gary Blau joined the faculty as Visiting Industrial Professor. Dr. Blau is a graduate of the University of Waterloo (Canada) with a PhD from Stanford University. Over a thirty year career with Dow and DowElanco, he achieved company-wide and national recognition for his accomplishments and expertise in applied statistics, mathematical model building for engineering systems, and risk analysis. Named a Dow Corporate Fellow in 1993 he received the Computing Practice Award of the AIChE at the 1997 Annual Meeting. In Spring 1998 he taught the undergraduate statistical modeling course and expects to offer a graduate course in risk analysis and applied statistics in the fall. He is an active participant in the Computer Integrated Process Operations Consortium (CIPAC), a collaborative research effort between a number of major corporations and the process systems engineering faculty of the School.

Late in 1997, Professor Jay Lee accepted an appointment in our School as Associate Professor, effective August 1998. Professor Lee earned the PhD at the California Institute of Technology in 1991, working under the direction of Professor Manfred Morari. He has served on the faculty of Auburn University, advancing to the rank of Associate Professor. He has held visiting appointments at DuPont Central S&E, the University of Washington, and Seoul National University. Professor Lee has established an outstanding research record in control relevant process modeling and identification as well as model predictive control with applications to pulp digester and batch polymerization reactor control. He has been recognized with an NSF National Young Investigator Award, the Auburn Alumni Council Senior Research Award, and the Auburn Pulp & Paper Foundation Professorship. He will become the newest CIPAC participant.

The School expects the arrival in Summer 1998 of Dr. David Corti, who will begin an appointment as Assistant Professor. Dr. Corti is completing a postdoctoral position at UCLA where he has been working with Professor Howard Reiss in the Department of Chemistry and Biochemistry. Dr. Corti, a graduate of the University of Pennsylvania, received the PhD at Princeton University working under the direction of Professor Pablo Debenedetti. His research involves computation methods for the study of the thermodynamic properties and behavior of liquids under temperature and pressure extremes, molecular theories of vapor phase nucleation, and statistical mechanics of nucleation and adsorption phenomena.

In September 1997, Professor Frank Doyle resigned from Purdue University to accept a position at the University of Delaware. Professor Doyle had joined the faculty in Fall 1992, advancing to the rank of Associate Professor with Tenure. Professor Hilary Lackritz completed a one year leave of absence and resigned from the faculty in Spring 1998. As a result of changes in her family circumstances, she found it necessary to accept a position with a research firm in the San Francisco Bay Area. She continues on the faculty in an Adjunct role, collaborating with Professor Caruthers in the polymer materials domain. In Spring 1998, the promotion of Professor Joseph Pekny to the rank of Full Professor was approved by the Board of Trustees, effective August, 1998. Professor Pekny, who joined the Purdue faculty in January 1990, has developed a nationally recognized research program in combinatorial optimization methods with applications in process planning, scheduling, and design.

Professional Recognition

Among the recognitions achieved by the faculty during the past year, Professor Ron Andres was appointed Editor of a newly launched publication, the Journal of Nanoparticle Research. He joins the four other faculty who currently serve as editors of research journals: Professor Delgass (Journal of Catalysis), Professor Peppas (Biomaterials), Professor Reklaitis (Computers & Chemical Engineering), and Professor Wankat (Separation and Purification Methods).

Professor Jochen Lauterbach was named a 1998 NSF CAREER Award winner. This is a four year grant which provides very flexible research funding for his work on the chemistry of polymer films on metal surfaces. Professor Nicholas Peppas was elected Fellow of the American Physical Society, High Polymer Physics Division. Professor Eva Sevick-Muraca was elected Fellow of the American Institute of Medical and Biological Engineering. She joins several Purdue ChE faculty, including Professors Peppas, Ramkrishna, and Tsao, who hold that distinction.

Professional Activities

The faculty continues to be very active in professional societies and governmental scientific advisory entities.

Professor Basaran was appointed to the Steering Committee for the 9th International Coating Science and Technology Symposium held in Newark, Delaware, May 1998, and to the EPA Spray Drift Task Force Panel, in December 1997. Professors Blau and Pekny are serving as co-chairs of the Third International Symposium on Foundations of Computer Aided Process Operations. This major conference in the operations field held once very five years will take place in Snowbird, Utah, in July 1998. Professor Caruthers continues his appointment on the NRC Standing Committee on the Program and Technical Review of the US Army Chemical and Biological Defense Command. Professor Greenkorn serves on the Global R&D Advisory Committee of the Council of Competitiveness and on the Board of Governors for Argonne National Laboratory. Professor Peppas served on the Organizing Committee of the 5th European Controlled Release Meeting (Netherlands). Professor Sevick-Muraca was appointed to the NIH Diagnostic Imaging and Radiology Study Panel. Professor Sinclair served on the Conference Scientific Committee for Fluidization IX (May 1998).

Professor Sevick-Muraca was named to the Editorial Board of the Journal of Biomedical Optics and continues to serve as Associate Editor of Photochemistry and Photobiology. Professor Sinclair was appointed to the Editorial Advisory Board of the Journal of Powder Technology, one of the premier archival journals in the particulate systems domain.

Collectively, the faculty chaired sixteen sessions at conferences, led or served on the organizing committees of seventeen conferences, and participated in nine expert panels. At the Annual AIChE meeting alone, the faculty chaired nine sessions and authored thirty-four presentations. Professor Peppas was organizer of the topical conference on Biomaterials at that meeting. Moreover, the session which Professor Sinclair chaired received the Best Session Award from the Institute. Prof. Basaran chaired a session on Drops and Bubbles at the American Physical Society Meeting and co-organized the Purdue Coatings Systems Research Center Symposium. Professor Sevick-Muraca served as general chair for the Optical Society of America Topical Meeting for Biomedical Optical Spectroscopy and Diagnostics, and as session chair at the Gordon Research Conference on Lasers in Medicine and Biology and at the Fourth Annual Meeting of the Frontiers of Engineering Symposium of the National Academy of Engineering. Professor Venkatasubramanian was a member of the International Program Committee for the 5th IFAC Symposium on Dynamics and Control of Process Systems (Greece).

The faculty are in high demand as lecturers and speakers at technical forums around the world, collectively giving 75 invited lectures and seminars. Among these, Professor Andres was invited speaker at the Gordon Conference on Clusters, Nanocrystals, and Nanostructures and at the NSF Workshop on Materials Design and Processing through Self-Assembly. Professor Delgass presented seminars at the Universities of Auckland and New South Wales. Professor Franses was invited speaker at the ACS Colloid Symposium in honor of Prof. D. Wasan. Professor Lauterbach presented seminars at Northwestern University and at the Ford Scientific Laboratory. Professor Pekny gave the keynote lecture at the Lilly Worldwide Modeling Conference and was invited speaker at the Mitsubishi Chemical Corporation Mini-Symposium on Modeling and Optimization. Professor Ramkrishna served as plenary lecturer at the Golden Jubilee International Conference of the Indian Institute of ChE, New Delhi, in December 1997, and presented a seminar at Rutgers University as part of the Merck Distinguished Lecture Series. Professor Reklaitis gave the Texas Distinguished Faculty Lecture in the ChE Department at the University of Texas, Austin. Professor Sevick was invited speaker at the International Conference on Methods and Applications of Fluorescence Spectroscopy (Berlin) and at the Engineering Foundation conference on Advances in Optical Techniques for Medicine and Surgery. Professor Sinclair was invited lecturer at the NSF Workshop on the Flow of Particulates and Fluids and at the Symposium honoring the retirement of Professor Roy Jackson. Professor Venkatasubramanian was invited speaker at the Gordon Research Conference on Quantitative Structure-Activity Relationships and at the O'Conner Process Safety Center Symposium, Texas A&M University. Professor Wang was invited plenary lecturer at the Brazilian Adsorption Society Meeting. Professor Wankat presented the Phillips Distinguished Lecture at Oklahoma State University and presented the ASEE Union Carbide Lectureship Award Lecture at the ASEE Chemical Engineering Faculty Summer School.

Staff Affairs

Staff Appointments

Over the past academic year, the School has experienced a number of staff changes which have resulted in seven new staff appointments. This represents an unusually high 30% turn-over of our staff. First, in anticipation of the retirement of Katie Eckman, our long-term Undergraduate Program Administrator, the School was fortunate to attract Janet Siebenthal, an experienced and highly regarded counselor in the Freshman Engineering Department. Mrs. Siebenthal joined the School in August 1997. Katie has continued in the Undergraduate Office at a half-time level over the past academic year so as to facilitate an effective transition. She expects to retire officially in October, 1998.

Also, in Summer 1997, our Computer Systems Manager, David Carmichael, resigned after over eight years in that position to take a promotion as User Services Manager with the Engineering Computer Network organization, His replacement, who assumed the position in August, was Steve Plite. Mr. Plite has a computer science background and extensive industrial experience as systems manager, most recently at the Weyerhaeuser Technical Center.

At the end of April, 1998, Hannah Moore, the School's Business Office Manager for over four years, accepted a promotion to a fiscal analyst position in the Development Office of the University. Diane Martin, who has a degree in management and previous experience in accounts administration at Purdue, will fill this position in August, 1998. Also, Hardie Davidson, who served as Purchasing and Reimbursements Clerk in the Business Office, graduated from Purdue in May and announced plans to commence with graduate studies at another university in Fall 1998. In anticipation of Ms. Davidson's departure at the end of the summer, a search was launched for her replacement so as to allow for an overlap training period. It is anticipated that Sheila Foster, who has over ten years experience as accounting clerk in the logistics business, will join the School.

Also in June, Karen Schneider, who served as Information Systems Operator and Assistant Cooperative Education Program Coordinator in the Undergraduate Office, accepted a new position in Forestry. Sandy Hendryx, who has extensive experience in supporting student counseling and registration activities in the Freshman Engineering Department, will join our School, effective August, 1998. Concurrently, a search to fill the position of Information Processing Systems Operator, which had been vacant for an extended period of time was initiated. Marcella Maynard accepted the position, effective at the end of July. Marcella has had extensive information processing experience with an insurance firm in the Lafayette area.

While all of the above described staff changes involved existing positions, in Spring 1998, the School created a new position to lead the School's development and alumni relations activities. The position has the title of Associate Director of Development and Alumni Relations, Chemical Engineering-based. Dr. Bettina McConnell started in that position on June 1, 1998. She had very successfully served in development functions with the Krannert School of Management for over a decade and thus brought extensive experience and knowledge of such activities to our School. She will focus particularly on major gift development.

Finally, in Fall 1998 the School plans to make two additional staff changes. First, using the funds generated from the newly instituted engineering differential fee paid by our students, we expect to add a staff member who will assist Steve Plite in providing desktop computer support. That position will be created and filled in Fall 1998. Furthermore, Kenny McGlothlin, who has for ten years been highly effective as demonstration assistant in the instructional laboratory of the School, has announced his intent to retire at the end of calendar 1998. In the fall, Dr. Wayne Muench, Director of Instructional Laboratories, will launch a search for Kenny's replacement.

Feedback Evaluation Process

As one of the action items identified in our Strategic Plan and in cooperation with Mobil Oil Corporation, the School launched the implementation of a 360 Feedback Evaluation Process. The purpose of this tool is to help the staff in improving its performance in working with students, faculty, and other staff as well as to improve the effectiveness of the faculty in working with staff. A detailed questionnaire was developed by a cross-functional team facilitated by consultants funded by Mobil. The questionnaire will be administered to selected students, faculty, and staff in early Fall 1998, after appropriate training in the goals, objectives, and desired outcomes of the program. Personnel Services will be monitoring this initiative as a pilot activity which, if successful, would be available for adoption by other units in the University. Personnel Services will also participate in the pre- and post-evaluation training activities so that in the future the 360 process can be supported internally by that organization rather than by outside consultants.

Graduate Education and Research

Research Productivity

The research productivity of the faculty as measured in expenditures, proposal activity, publications, and conference presentation continues at high levels. The School was ranked 10th in total research expenditures (Chemical & Engineering News, Sept 1997) among peer ChE departments. Overall research expenditures from extra-mural sources increased by 5% to $4.8 million. It is noteworthy that while over the previous five year period expenditures of university budgeted funds have increased by only 19%, expenditures of externally secured funds have increased by nearly 34%. Proposal activity has increased substantially over the past year in all categories: number of submissions, dollar value of submissions, number of awards, and dollar value of awards. The faculty submitted 63 proposals in 97-98 vs 37 in 97-97 and the dollar value of submissions increased to $12.2 million vs $7.7 million in the previous year. Awards increased to 81 funded projects in 97-98 vs. 64 in 96-97 and the dollar value of new awards increased to $3.5 million vs $2.6 million in the previous year. These increases attest to the strong entrepreneurship of the faculty and the excellent support that the staff has given to the faculty in generating and executing research projects.

The tangible results of the grants and contracts funding include 261 papers in print or in press, compared to 275 in the previous year. The research groups contributed nearly 120 meeting presentations, compared to 134 in the previous year. Invited lectures and seminars totaled 75, a decline from the all-time high of 93 reported in 96-97. These presentations and lectures involved 18 of the 22 faculty, thus constituting an

average of 11 per year among these faculty. This attests once again to the high level of professional involvement of the faculty.

Graduate Enrollment

In the 1997-98 academic year, the School graduated 20 PhD and 16 MS degree candidates, a slight decrease from the 22 and 18, respectively in the previous year. While comparative figures for this academic year are not yet available, the School was 4th in PhD awards and 6th in MS awards in 1996-97. Indeed, over the past five years our School has been 4th in total PhD awards in ChE in the US.

The School has been controlling graduate admissions at a lower level than was the case in the early 1990's, with the objective of increasing the quality of the pool admitted to the PhD program. Thus, the entering class in Fall 1997 consisted of 20, including 15 with undergraduate degrees from US institutions and four women students. However, with the very strong job market of the past two years, a larger than normal number of students have elected to terminate graduate education at the MS level, causing our total fall full-time graduate enrollment to decline below 100 for the first time since 1984. Consequently, admissions have been increased somewhat for Fall 1998: the entering class is expected to number 26, including six women students. Fall 1998 total graduate enrollment is expected to be near 100.

Graduate Research Symposium

The Graduate Student Organization of the School convened the sixth annual Graduate Research Symposium on August 21, 1997. The Symposium was chaired by Aaron Cote, President of GSO, assisted by an organizing committee of nine GSO members and officers. The Symposium featured 16 oral presentations, organized into two parallel tracks, as well as 22 poster presentations. The Symposium drew an audience of 40 industrial representatives from 21 different companies. These representatives served as jury for the selection of the best presentations. The winners were as follows: Session 1 & Session 2. First Place, Steve Honkomp, Ted Pirog. Second Place, Nancy Irwin, Michael Ernest. The Seventh Annual Symposium, scheduled for August 20, 1998, will be chaired by Eric Stangland. To date, 22 companies have agreed to sponsor the Symposium. The steady growth of industrial interest in the Symposium attests to the high quality of the program and the professional manner in which GSO has organized the event.

GAANN Fellowships

In June the School was informed by the Department of Education that it had successfully competed for a block grant of seven graduate fellowships under the Graduate Assistance in Areas of National Needs program. The three year fellowships, which provide stipends of $15,000/yr plus a travel and supplies allowance, are intended for the support of nontraditional graduate students. This is the fourth such grant which the School has received. The third grant terminates in August, 1998. The GAANN program is administered by Professor Jim Caruthers, Graduate Program Director.

Undergraduate Education

Awards

The Purdue student chapter of AIChE participated in the Midwest Regional Student Conference held in April at the University of Illinois, Urbana campus. Purdue students, Julie Wright and Upma Sharma,

won first and third prize, respectively, in the student research paper competition. As a result, Julie Wright, whose research advisor is Professor Lauterbach, will have the opportunity to present her work at the Miami Beach Annual AIChE meeting and compete for a national AIChE award.

A seven member team consisting of sophomores, juniors, and seniors, advised by Professor Lauterbach, was selected to participate in the NASA Microgravity Program. The team members were Trisha Beutien, Brad Ecker, Cassandra Forthofer, Hilary Grinstead, Jennifer Ralston, Nicholas Saddah, and Amanda Schreiweis. Purdue was the only university that had two teams selected, one from Aero-Astro and the other the ChE team. The ChE team designed and constructed a reaction-diffusion experiment involving the Belousov-Zhabotinskii reaction and successfully flew the experiment at the end of March, 1998 in Houston. The team's effort was widely reported by the national and local press as well as TV. The interesting findings will be reported in a scientific paper which is in preparation.

The high quality of the instructional programs of the School is the result of the combined efforts of the faculty, teaching assistants, and the very able support staff. The critically important contributions of the graduate teaching assistants were recognized through the 1998 Purdue University Magoon Awards which were presented to Steve Honkomp, Karen Greene, Praveen Gunaseelan, Steve Richter, and Will Walters. It is noteworthy that this is the third time that Steve Honkomp has won this recognition. Timothy Pletcher was selected by the seniors for the Award of Teaching Excellence in the Undergraduate Laboratory. In addition to suitable recognition mementos, the award recipients receive a cash prize of $500.

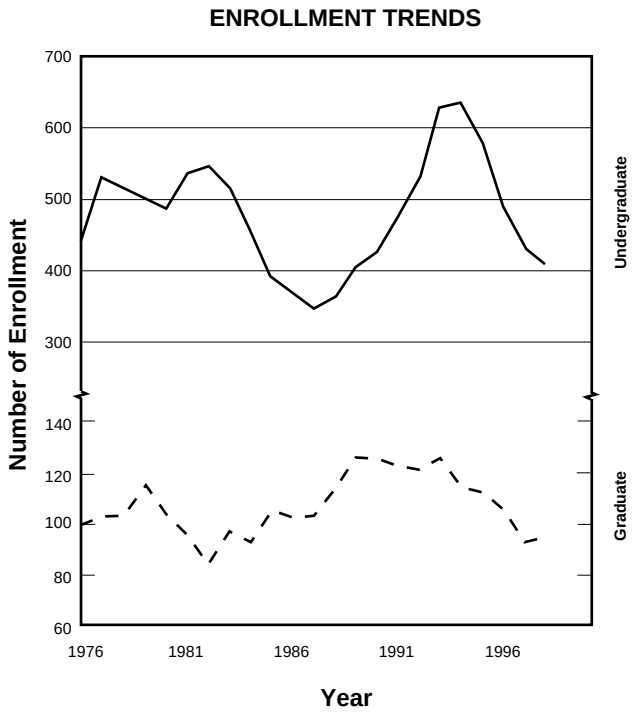
The 1998 student awards were voted by the faculty and presented at the awards banquet held on April 30, 1998. The awards for outstanding junior students were presented as follows: Steven Craig Award - Cassandra Forthofer; George T. Tsao Award - Roger Hoover

The awards for seniors were as follows: The Craig Outstanding Senior Award (managed by AIChE) - Tom Manske, The Bruce Wilson Award (managed by Omega Chi Epsilon) - Bryan Comstock, Lottes Award - Kevin Rabinovitch, A.I. Chemists Award - Ben Voss. 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 eighth semester senior process design course, was won by the design team of Robert E. Cowden, Herman Gunawan, Steven J. Tomory and Bryan D. McVicker. The second place team was that of Elizabeth K. Boswell, Mariah C. Deguara, Robert B. Ecker and Scott A. Liffick. The names of the recipients of all of these awards are recorded on the associated award plaques located in the School's permanent display case.

Enrollment Trends

The School continues to graduate the largest numbers of BS chemical engineers among all ChE departments in the US. Indeed this has been the case for over ten years. In the 1997-98 academic year, counting August, December, and May graduations, 150 BS ChE's were awarded, including 135 in May, 1998. These numbers are a substantial reduction from the 186 and 184 total BS awards which occurred in the previous two academic years. The decline in ChE majors is the result of several factors: the grade point cap on admissions from Freshman Engineering

into ChE which has been in place for several years, the general reduction in engineering admissions, as well as the shift in student interest to areas such as computer engineering and computer science. Advancement of students from the Freshman Engineering program to ChE had declined from 231 in 1993 to a low of 104 in 1996 but has now increased to 144 in 1998. The increases of the past two years are most likely a consequence of the very strong job market and highly publicized starting salaries for ChE's. As a result of these factors, our program has undergone the enrollment swings shown in Figure 1. Note that the totals shown include only those students who have advanced beyond the first year common Freshman Engineering program.



As can be seen, the Fall 97 enrollment of 430 is expected to decline to 400 in Fall 1998. However, since 1999 advancements for FrE are expected to exceed the 1999 senior class, we expect overall enrollments to climb again by Fall 1999.

ChE Student Advisory Council

One of the action items of the Strategic Plan for the School, adopted in Fall 1997, was the creation of a student advisory council. The Council charter was developed by the founding student group and approved by the Dean of Students Office in October 1997. The purpose of the Council is two-fold: to facilitate communication between ChE students, faculty, and administration and to take action to address student concerns and suggestions. The Council consists of 12 students including representation from sophomore, junior, and senior classes as well as representation from co-op students, AIChE student chapter, and the Omega Chi Epsilon honorary society. Council members are selected by the Council officers on the basis of an application and interview process. The Council officers consist of a president, secretary, and treasurer. Becca Kopp, Class of '99, led the formation of ChE SAC. The first Presi-

dent of the Council was Cassandra Forthofer, Class of '99. The Council meets with the Head and Associate Head of the School each month and has undertaken a number of initiatives in the 1997-98 academic year. These include the implementation and execution of midterm evaluations of ChE undergraduate courses as requested by the faculty, the revitalization of the ChE Connections student-to-student mentoring program, the implementation of an all-school student survey to identify problems and opportunities in curriculum, facilities, and student-faculty relations, the organization of an open forum with the junior class held in Spring 1998, the initiation of an advising program for freshman interested in ChE, as well as the organization of a Thank-a-thon in which thank-you calls were placed to alumni who had made financial contributions to the School in the past year.

Facilities Development

For the 1997-99 biennium, the School was allocated $380,000 for the initial phase of a multiphase renovation of the Undergraduate Laboratory. The renovation plan calls for a $1 million investment to completely remodel the entire 4500 sq.ft. facility. This is to be paralleled by a comprehensive refurbishment of the inventory of experiments and associated instruments. During the 1997 Christmas break, old plumbing and utility lines were removed, and beginning in May 1998 the construction of a loft was initiated in the high bay area of CHME 10. The construction of the loft and complete renovation of the high bay area is expected to be completed by the start of Fall 1998 semester. Residual funds from the allocation together with funds which may be allocated in the 1999-2001 biennium will be used to complete the remodeling of the remaining portion of CHME 10. The renovation of the CHME 11 portion of the lab will await fund allocation in 2001. To address the renewal of the complement of lab experiments the School has launched a multi-year fund-raising campaign among alumni and corporate sponsors in Winter 1997.

With the 1998-99 academic year budget, the Board of Trustees of the University approved the imposition of a differential engineering fee of $100/semester as well as an increase in the technology fee which had been adopted in the previous year. As a consequence, the School was able to compete for funds for an extensive instructional computing upgrade. As a result of successful proposals developed by Professor Pekny, chair of our Computing Committee, and Steve Plite, the School obtained $270,000 in funding. When combined with matching funds of $50,000 derived from gifts, the total project funding will be sufficient to allow complete replacement of 50 desk top computers in the Undergraduate Computing and Process Systems Engineering Laboratories, the two departmental file and computer servers, some of the shared printing facilities, as well as the required software. This acquisition will also serve to initiate a transition of departmental computing facilities from a predominantly Unix and Mac OS environment to a predominantly Widows NT environment. It is anticipated that this conversion will be completed by June 1999.

For Fall, 1998, the University announced that two of the smaller of the three classrooms in CHME will be remodeled. The renovation will entail new air handling, lighting, and A/V equipment addition, including the installation of PDN wiring and computer projection equipment. This renovation is to be completed in time for the January 11, 1999 start of classes.

Industrial and Alumni Relations

Industrial Advisory Board

Over the past ten years the School has built and fostered a unique collaborative program with industry called New Directions in Chemical Engineering. Through this valued partnership, leading corporations, who rely on chemical engineering talent as a key resource, work directly with the School to advance and improve the education and professional preparation of ChE's who will meet the needs of industry in the 21st century. Members influence the direction of education and training of students, derive preferential access to potential employees, and have input and access to the School's research programs.

During the past year, the program has been refocused as a result of the creation of a Strategic Plan for the School for the period 1997-2002. The final version of the Strategic Plan, which was developed by the faculty working in close collaboration with the Executive Committee of the New Directions program, was presented at the Annual Meeting of the full Industrial Advisory Council of the program which was convened September 11-12, 1997. The vision established under this Plan is that the School will be recognized as the premier source of well-educated and well-prepared chemical engineers in the world. The plan sets specific goals, strategies, action items, and metrics in five areas: graduate program, undergraduate program, faculty, technical infrastructure, and administrative infrastructure, and outlines the resource requirements for meeting those goals. During the discussions and break-out sessions held during the annual meeting, mixed groups composed of industry representatives, faculty, staff, and students worked on specific action items that would be pursued together with our industrial partners.

The Executive Committee, consisting of eight senior executives, is chaired by Bill Wishlinski, VP Engineering and Construction, Amoco. During the past year, Donald Orr, Senior VP, Air Products and Chemicals, a long-term member of the Committee, retired and was replaced by Robert Davis, also of Air Products. After the Annual Meeting of the Council, the Executive Committee met twice during the year: December 10, 1997, in Houston, and May 22, 1998, in Fairfax, Virginia, and conducted several teleconferences. The December meeting focused principally on three items: discussion of key tactical issues resulting from the Strategic Plan, brainstorming on the mission and functions of the Industrial Advisory Council and the Executive Committee which properly align these entities with the Strategic Plan, and discussion of strategies for meeting the space needs of the School, one of the pivotal resource requirements for achieving the goals of the Plan. The May meeting served to develop the framework for a possible capital campaign for the School, to develop a plan for launching a membership campaign for New Directions, to reexamine the New Directions Committee structure to align it with the goals of the Strategic Plan, and to outline the agenda for the Annual Meeting of the Industrial Advisory Council to New Directions, which is scheduled for October 2-3, 1998. Given that the university decision on how best to meet the future space needs of the School has been delayed, the Executive Committee has focused its attention for the next academic year on the membership campaign.

Alumni Awards

The School is delighted that one of its accomplished alumni was successful in the rigorous, multi-level evaluation and selection process for candidates for the Honorary Doctorate. Richard Hazleton, BS' 65,

Chairman of Dow Corning, was awarded the degree, Doctor of Engineering, Honoris Causa, during the Engineering Commencement exercises held on May 17. Dr. Hazleton was a recipient of the Distinguished Engineering Award in 1993.

The School also succeeded in advancing the nominations of Charles Kline, BS'60, and William E. Smith, III, BS'69, for 1998 Distinguished Engineering Alumnus Awards. Mr. Kline is President, Equate Petrochemicals, a joint venture of Union Carbide with Kuwait, while Mr. Smith is Executive Director for Engineering and Manufacturing of Eli Lilly & Company. These ChE alumni were among the ten member, engineering-wide group who were presented for awards during the Distinguished Engineering Alumnus Convocation which was held on campus on April 24, 1998.

The faculty voted two of our alumni the departmental Outstanding Chemical Engineer Award for 1997: Guy Camarata BS'60, Executive Vice President and Director, Caltex, and Robert McNeeley, BS'67, President, Reilly Industries. The award presentations are scheduled to take place, October 29, 1998, the Thursday before the annual President's Council Weekend.

Faculty Summary

Lyle F. Albright

**1955*

Professor Emeritus

Degrees

BS, University of Michigan, 1943

MS, University of Michigan, 1944

PhD, University of Michigan, 1950

Interests

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

High polymers and polymerization

Gasification and liquefaction of coal

Pulping of wood chips for paper production

Publications

Albright, L.F., "Polyethylene: The Versatile Plastic. Part II: Production of HDPE's and LLDPE's with Slurry and Solution Processes." *Polymer News , 22, No. 8*, 281 (1997).

Albright, L.F., "Polyethylene: The Versatile Plastic. Part III: Production of HDPE's and LLDPE's with Gas Phase Processes Plus General Conclusions." *Polymer News , 22, No. 11*, 393 (1997).

Albright, L.F., "Comments on Supercritical Phase Alkylation Reactions on Solid Catalysts: Mechanistic Study and Catalyst Development," *Ind. Eng. Chem. Research, 37*, 296, (1998).

Albright, L.F., "Updating Alkylate Gasoline Technology," *CHEMTECH 28, No. 6*, 40-46, (1998).

Albright, L.F., "Improving Alkylate Gasoline Technology," *CHEMTECH 28, No. 7*, 46-53, (1998).

Editorial Boards

Encyclopedia of Chemical Processing and Design, 1976-present

Polymer News, 1995-present

Invited Lectures

Speakers Bureau of American Institute of Chemical Engineers

Symposium at Dallas ACS Meeting in March 1998 honoring A. R. Goldsby.

** Year of joining the faculty.*

Ronald P. Andres

1981

Engineering Research Professor

Degrees

BS, Northwestern University, 1959

PhD, Princeton University, 1962

Interests

Ultrafine particles

Nanostructured materials

Nanoelectronic devices

Catalysis

Scanning Probe Microscopy

Research Areas

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

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

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

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

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

Publications

R.A. Crane, J.T. Matthews, and R.P. Andres, "Synthesis of Oxide Coated Metal Clusters," *Mater. Res. Soc. Symp. Proc.*, 457, *(1997).*

R.P. Andres, S. Datta, D.B. Janes, C.P. Kubiak, R. Reifenberger, "The Design Fabrication and Electronic Properties of Self-Assembled Molecular Nanostructures," *Handbook of Nanostructured Materials and Nanotechnology* (ed. H.S. Nolwa) Academic Press (1998).

Meeting Presentations

"AFM Characterization of a Fiber-Matrix Interface Using a Carbon Nanotube Modified Probe," Materials Research Society, Boston, MA, December 1997.

"Self Assembly of a Two-Dimensional Superlattice of Electronically-Linked, Nanometer-Diameter, Metal Clusters," Materials Research Society, Boston, MA, December 1997.

"Fabrication of a 2D Patterned Network of Gold Clusters Linked by Molecular Wires," American Physical Society, Los Angeles, CA, March 1998.

"AFM Imagining of Nanometer Scale Objects in Water," American Physical Society, Los Angeles, CA, March 1998.

"Design and Characterization of a Distributed Arc Cluster Source for Nanoparticles Synthesis," American Association for Aerosol Research, Cincinnati, OH, June 1998.

Invited Lectures

"Synthesis of a Two-Dimensional Superlattice of Covalently Linked Gold Clusters," Gordon Conference on Clusters, Nanocrystals, and nanostructures, Plymouth, NH, July 1997.

"Networks of Molecularly Linked Metallic Nanoclusters: Potential as Chemical/Biological Sensors, ERDEC, Edgewood Arsenal, MD, August 1997.

"Technology Leadership: Educational Value of Discovery Directed Research," Purdue Board of Trustees, November 1997.

"Designing Nanostructured Materials Through Molecular and Subunit Architecture," NSF Workshop on Materials Design and Processing at the Nano-and Mesoscales through Self-Assembly, Washington, DC, January 1998.

"Fabricating Functional Nanostructures from Metal Quantum Dots," Physics Department Seminar, Carnegie Mellon University, Pittsburgh, PA, March 1998.

"Interdisciplinary Nanoelectronics Research at Purdue," President's Academic Review, Schools of Engineering, April 1998.

Osman Basaran

1995

Professor

Degrees

BS, Massachusetts Institute of Technology, 1978

PhD, University of Minnesota, 1984

Interests

Computational fluid dynamics (CFD) and finite element analysis

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

Interfacial phenomena; surface and bulk rheology

Ink-jet printing and atomization coating

Biochips, MEMS, and miniaturization

Electric field-enhanced separations

Research Areas

The research program is motivated by practical applications ranging from ink-jet printing to miniaturization of bioanalytical instrumentation to separations. In particular, the group is involved in developing the scientific underpinnings of applications including but not limited to

- so-called discontinuous coating flows such as ink-jet printing, atomization coating, spray painting, and crop spraying
- electrically enhanced solvent extraction and distillation
- measurement of interfacial and bulk rheological properties
- micro fluid dynamics of flows arising in biochip processors and devices that do “biochemistry on a chip.”

In ink-jet printing, atomization coating and painting, and crop spraying, two central problems are the generation of drops from a nozzle and the deposition of drops that are thereby generated on a suitable substrate. Both of these problems are under study using computational and experimental techniques. Of particular interest to the group in these studies are the effects of surfactants and dynamic surface tension (DST), non-Newtonian rheology and shear-thinning behavior of liquids, and viscoelasticity and extensional viscosity of liquids. The group has pioneered and continues to develop novel finite element algorithms for determining the large deformation and breakup of liquid drops. An area of current emphasis is following the dynamics through several breakup events and porting algorithms and codes to parallel machines. On the experimental side, the group, which has pioneered direct visualization of drop dynamics events with a time resolution of fractions of

a millisecond (or hundreds of microseconds), has recently started pushing the envelope down to tens of nanoseconds to a few microseconds.

In separations, two distinct thrust areas are under scrutiny. The first is the use of electric fields in enhancing the efficiency of separations such as solvent extraction. Here interest is focused on how electric fields can be used to produce mono-sized drops and eliminate satellite droplets. Progress in this effort is being expedited by the use of a two-component Phase Doppler Anemometer that is capable of measuring the size and two components of the velocity of drops in an electrospray. In parallel to PDA, high-speed visualization and computation are being utilized to gain insights into drop formation phenomena. The other thrust area is focused on fluid mechanics of distillation, which has heretofore been studied through empiricism rather than engineering science. The goals here are to gain a better understanding of both the global flows on distillation trays and bubble formation in shear flows.

Novel equipment has either been built recently or is in the process of construction to measure dynamic surface tension and extensional viscosity. The Purdue growing drop apparatus for measuring DST, which is now operational, can probe surface tension variations on time scales as short as 1/12th of a millisecond. The new Purdue extensional rheometer should be operational within the next six months. These novel pieces of equipment allow the scientist/engineer to measure surface and bulk properties on time scales of relevance to industrial practice.

There is great interest in miniaturizing devices used for bioanalysis and coming up with efficient and accurate techniques for DNA analysis and sequencing. A common thread in these life science applications is the manipulation of ultra-small volumes of liquids, such as in dispensing microdoses of solutions of oligonucleotides onto surface-treated substrates or in pumping blood or reagents through micron-size channels. Several such problems are being studied in collaboration with various industrial companies.

Publications

Wilkes, E.D. and Basaran, O.A. 1997. "Forced oscillations of pendant drops." *Phys. Fluids 9*, 1512-1528.

Wham, R.M., Basaran, O.A., and Byers, C.H. 1997. "Wall effects on flow past fluid spheres at finite Reynolds number: wake structure and drag correlations." *Chem. Eng. Sci.* 52, *3345-3367*.

Ambravaneswaran, B., Kim, J. S., Zhang, X., and Basaran, O. A. 1997. "Stretching and Breakup of Liquid Threads in Drop Formation: Effects of Surfactant Additives and Electric Fields." Proceedings of ILASS-Americas (1997), pp. 329-333.

Zhang, X. and Basaran, O. A. 1997. "Impact of Surfactant-Laden Drops with a Substrate in Atomization Coating and Crop Spraying." *Proceedings of ILASS-Americas* (1997), pp. 150-154.

Invited Lectures

Basaran, O.A., "Drop Formation: Effects of Electric Fields, Viscous Forces, and More," Engineering Sciences and Applied Mathematics Colloquium- Departmental Seminar, Northwestern University, Evanston, Illinois, February 2, 1998.

Basaran, O.A., "Drop Dynamics and Interfacial Phenomena in Crop Spraying and Related Problems," Dow Elanco Corporation, Indianapolis, Indiana, July 15, 1997.

Basaran, O.A., "Dynamics of Drop Formation and Impact: Effects of Electric Fields, Surfactants, and Viscous Forces," Packard Instrument Company, Downers Grove, Illinois, January 27, 1998.

Meeting Presentations

Ambravaneswaran, B. and Basaran, O.A., "Surfactant Effects on the nonlinear Deformation and Breakup of Stretching Liquid Bridges," AIChE 1997 Annual Meeting, 16-21 November 1997, Los Angeles, California.

Kim, J. S. and Basaran, O.A., "Effects of Tangential and Normal Electric Fields on the Deformation and Breakup of Stretching Liquid Bridges," AIChE 1997 Annual Meeting, 16-21 November 1997, Los Angeles, California.

Notz, P.K. and Basaran, O.A., "Dynamics of Drop Formation in an Electric Field," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

Wilkes, E.D. and Basaran, O.A., " Computational Analysis of Dynamics of Drop Formation," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

Kim, J.S. and Basaran, O.A., "Effects of a Tangential Electric Field on the Deformation and Breakup of a Stretching Bridge of a Perfectly Insulating Liquid Bridge," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

Ambravaneswaran, B. and Basaran, O.A., "Effects of Insoluble Surfactants on the Nonlinear Deformation and Breakup of a Stretching Liquid Bridge," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

Yildirim, O. and Basaran, O.A., "Deformation and Breakup of Non-Newtonian Liquid Bridges Undergoing Uniaxial Extension," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

Chaired Conferences/ Symposia

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

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

Session Chair, "Drops and Bubbles (Session Cf)," 50th Annual Meeting of the Division of Fluid Dynamics (DFD) of the American Physical Society (APS), 23-25 November 1997, San Francisco, California.

NASA, Microgravity Fluid Physics, Interfacial Phenomena Panel. 29-30 May 1997, Washington, D.C.

US DOE Environmental Management Science Program, Separations Chemistry Panel. 5-6 June 1997, Washington, D.C.

EPA, Spray Drift Task Force Panel. 11 December 1997, Washington, D.C.

Facilitator, Panel Discussion on "Deposition and Coatings," 10th Annual Conference on Liquid Atomization and Spray Systems (ILASS), Ottawa, Canada, 18-21 May 1997.

Member Steering Committee, 9th International Coating Science and Technology Symposium, 17-20 May 1998, University of Delaware, Newark, Delaware.

Chairperson, Deposition and Coatings Technical Committee, 10th Annual Conference on Liquid Atomization and Spray Systems, ILASS Americas '97, Ottawa, Canada, May 1997.

Co-organizer of Purdue Coatings Systems Research Center Symposium, 19 March 1998, Purdue University, W. Lafayette, Indiana.

Gary E. Blau

1998

Visiting Industrial Professor

Degrees

BASc, University of Waterloo, 1964

MSc, Stanford University, 1966

PhD, Stanford University, 1968

Interests

Mathematical Model Building of Engineering Systems

Operations Research

Optimization

Applied Statistics

Environmental Systems

Uncertainty / Risk Analysis

Research Areas

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

Publications

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

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

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

Blau, G.E., "A Systems Engineering Approach to New Product Development," *CAST Communications*, *20*, 2, (1997).

Invited Lectures

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

"The Optimal Design of Multiproduct Facilities using Combinometric Optimization," University of Waterloo, 1997.

"Future Directions for Math Modeling," Keynote Speaker, Lilly Conference on Statistical Modeling, Indianapolis, 1997.

"Treatment of Uncertainty in New Product Development," ETH Zurich, 1997.

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

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

Research Areas

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

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

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

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

Publications

D.H.S. Ramkumar and J.M. Caruthers, H. Mavridis and R. Shroff, "Computation of the Linear Viscoelastic Relaxation Sprectrum from Experimental Data," *Journal of Applied Polymer Science, 64, 2177, (1997).*

S. Krishnaswami, D. Ramkrishna, and J. M. Caruthers, "Statistical-Mechanically Exact Simulation of Polymer Conformation in an External Field," *Journal of Chemical Physics, 107,* 5929, (1997).

C.R. Novenario, J.M. Caruthers, and K.C. Chao, "Heat Capacity of Polymer Melts from the Polymer Chain-of-Rotators Equation of State," *Journal Applied Polymer Sci, 67*, 841-848, (1998).

Novenario, C.R., J.M. Caruthers, and K.C. Chao, "Chain-of-Rotators Equation of State for Polar and Non-Polar Substances and Mixtures, " *Fluid Phase Equilbria, 142*, 83-100, (1998).

Novenario, C.R., J.M. Caruthers, and K.C. Chao, "Vapor-Liquid Equilibrium of Polymer+Solvent Mixtures," *Ind. Eng. Chem. Res., 37*, 3142-3150, (1998).

Invited Lectures

"Thermoviscoelastic Models for Predicting the Time-Dependent Response of Engineering Polymers," GemFire Corp., Palo, Alto, CA, November, 1997.

Meeting Presentations

"Thermoviscoelastic Constitutive Models for Describing Enthalpy Relaxation in Amorphous Polymers," M.R. Hooker, P. Shirkhande and J.M. Caruthers, Society of Rheology, Columbus, OH October, 1997.

"Prediction of Three-Dimensional Deformations for Polymer Solids in the Glass Transition Region Using a Nonlinear Thermoviscoelastic Constitutive Equation," R.S. Chambers, J.M. Caruthers, and D.B.Adolf, Society of Rheology, Columbus, OH October, 1997.

"The Effect of Local Density Fluctuations on Volume Relaxation in the Glass to Rubber Transition Region," G.A. Medvedev, R. Bhatia, H.S. Lackritz, and J. M. Caruthers, Society of Rheology, Columbus, OH October, 1997.

"The Use of Generalized Strain Measures in a Thermoviscoelastic Constitutive Equation for Amorphous Polymers," P. Shirkhande, M.R. Hooker, and J.M. Caruthers, Society of Rheology, Columbus, OH October, 1997.

"A Thermoviscoelastic Constitutive Model for Describing the Melt Flow and Solidification for Amorphous Polymers," P. Shirkhande and J.M. Caruthers, Society of Rheology, Columbus, OH October, 1997.

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 rotational motion about the backbone 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

Novenario, C.R., J.M. Caruthers, and K.C. Chao, "Chain-of-Rotators Equation of State for Polar and Non-Polar Substances and Mixtures," *Fluid Phase Equilibria, 142,* 83-100 (1998).

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

Novenario, C., J.M. Caruthers, and K.C. Chao, "Heat Capacity of Polymer Melts from Polymer Chain-of-Rotators Equation of State," *J. Applied Polymer Science, 67,* 841-848 (1998).

Novenario, C., J.M. Caruthers, and K.C. Chao, "Vapor-Liquid Equilibrium of Polymer+Solvent Mixtures," *Ind. Eng. Chem. Res., 37,* 3142-3150 (1998).

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

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

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

infrared spectroscopy (DRIFTS) is used to study the interaction between the diol and the zeolite surface. Both the spectroscopic and kinetic measurements suggest that zeolite structure is important to activity, with MFI materials showing the highest rate and selectivity to MEK at mild temperatures. Lessons learned from these systems will be applied to other opportunities to replace liquid acids by solid acid catalysts.

Epoxidation of Olefins over Promoted Silver and Gold Catalysts: Silver is unique among the elements in its ability to catalyze the reaction of oxygen with ethylene to form ethylene oxide (EO) rather than the thermodynamically preferred product, CO_2. Silver is also known to catalyze epoxidation of butadiene to 3,4 epoxy 1-butene (EpB). Cs promotes catalysis of both reactions, but optimum formulations for the two systems are quite different. Studies of effects of Cs and support on Ag activity are now being followed by transient isotopic switch experiments, in which sudden replacement of $^{16}O_2$ with $^{18}O_2$ during steady state reaction allows us to quantitatively evaluate kinetically different oxygen pools on the surface of and in the catalyst. Previous work has shown that subsurface oxygen is a key ingredient of selective EO catalysts. We are interested to know the role of surface and subsurface oxygen species in EpB catalysis. Most recent studies of this system use Raman spectroscopy to probe the role of Cs.

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

Investigation of Spatially Patterned Catalytic Reactors: The theme of this collaborative work with Professor Ramkrishna is to enhance the performance of a primary reaction system by introducing an auxiliary reaction system catalyzed by a second catalyst. This enhancement may occur by alleviating an equilibrium constraint, removing a reaction inhibitor, “tuning” the reactant feed, or annihilating an environmentally hazardous by-product. The broad objective is to experimentally and theoretically study catalytic reactors with various types of spatial patterns intended to improve reactor selectivity and conversion. The patterns of interest, identified by their characteristic length scales, and are: (1) a well-mixed bed comprised of composite pellets containing both functionalities, (2) a well-mixed discrete bed containing different types of pellets with distinct functionalities, and (3) a spatially segregated bed alternating between layers of each distinct catalyst. More specifically, we seek to evaluate when each type of pattern will be most advantageous while generating a general methodology for properly orchestrating a pattern.

Preliminary calculations indicate that spatial patterns, in the absence of symmetry-breaking phenomena, hold great potential for improving the performance of many reaction systems and, therefore, may be attractive alternatives to traditional configurations. A fundamental understanding of these patterns may provide an avenue for greater optimization of dual-functional reactors thus maximizing conversion and selectivity to

Preliminary calculations indicate that spatial patterns, in the absence of symmetry-breaking phenomena, hold great potential for improving the performance of many reaction systems and, therefore, may be attractive alternatives to traditional configurations. A fundamental understanding of these patterns may provide an avenue for greater optimization of dual-functional reactors thus maximizing conversion and selectivity to desired products or minimizing the production of hazardous by-products.

Publications

Van Gruijthuijsen, L. M. P., G. J. Howsmon, W. N. Delgass, D. C. Koningsberger, R. A. van Santen, and J. W. Niemantsverdriet, "Structure and Reactivity of Bimetallic FeIr / SiO_2 Catalysts after Reduction and During High-Pressure CO Hydrogenation," *J. Catal, 170, 331-345 (1997).*

Lauterbach, J, S. White, Z. Liu, G. M. Bodner, and W. N. Delgass, "A Novel Laboratory Course on Advanced Chemical Engineering Experiments," *Chem. Engin. Education*, 260-265, Fall (1997).

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

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

Co-Editor

Journal of Catalysis

Invited Lectures

"Isotopic Transient Kinetic Studies of Ethylene Oxidation over Silver," Department of Chemistry, University of Auckland, Auckland, NZ, October 8, 1997.

"Selective Hydrogenation of Butyronitrile over Promoted Raney® Nickel Catalysts," Department of Chemical Engineering, University of New South Wales, Sydney, AU, October 13, 1997.

Meeting Presentations

"Selective Hydrogenation of Butyronitrile over Promoted Raney® Nickel Catalysts," S. N. Thomas-Prior, T. A. Manz, Z. Liu, S. K. Sengupta, T. A. Koch, W. N. Delgass, Organic Reaction Catalysis Society Meeting, New Orleans, LA, March 1998.

Roger E. Eckert

1964

Professor

Degrees

BS, Princeton University, 1948

MS, University of Illinois, 1949

PhD, University of Illinois, 1951

Interests

Statistical design of experiments

Flow properties of viscoelastic polymers

Mass transfer effect on reaction selectivity

Research Areas

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

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

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

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

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.

Publications

Akiti, T.T. Jr., L.D. Bircumshaw and R.E. Eckert, "Sequential Design Including Initial Experimental Runs For a Kinetic Study of Propylene Oxidation," *Canadian J. Chem. Eng,* 75, 238-244, (1997).

Albright, L.F. and R. E. Eckert, "New and More Rapid Methods to Determine Octane Numbers of Alkylates Produced in Refineries," *Oil & Gas J.*, (in press).

Akiti, Tetteh. T., Jr., and Roger E. Eckert, "Initial-runs Sequential Nonlinear Experimental Design Critieria Applied to Kinetic Modeling," *Ind. Eng. Chem. Res.*, (submitted).

Elias I. Franses

1979

Professor

Degrees

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

PhD, University of Minnesota, 1979

Interests

Interfacial Engineering - Thin Films - Mass Transfer

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

Adsorption and Transport of Lung Surfactants

Effects of Processing on Properties of Thin Organic Coatings

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

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

Research Areas

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

stability, and microstructure of these monolayers using radiotracer, optical, and infrared spectroscopic probes.

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

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

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

Publications

Pinazo, A. Seguer, J., Infante, M. R., Park, S. Y., and Franses, E. I., "Surface Properties of Aqueous Systems of New Nonionic Double-Chain Surfactants and Their Mixtures with DLPC (Dilauroylphosphatidylcholine)," *Colloids Surfaces A*, 126, 49-58 (1997).

Cho, D., Narsimhan, G., and Franses, E.I., "Adsorption Dynamics of Native and Pentylated Bovine Serum Albumin at Air-Water Interfaces: Surface Concentration/Surface Pressure Measurements," J. *Colloid Interf. Sci., 13*, 312-325, (1997).

Cho, D., Narsimhan, G., and Franses, E.I., "Interactions of Spread Lecithin Monolayers with Bovine Serum Albumin in Aqueous Solution," *Langmuir, 13,* 4710-4715 (1997).

Franses, E.I., Chang, C.-H., Chung, J.B., Coltharp, K.A., Park, S.Y., and Ahn, D.J., "Dynamic Adsorption and Tension of Spread or Adsorbed Monolayers at the Air/Water Interface," in *Micelles, Microemulsions, and Monolayers: Science and Technology,* Shah, D.O., ed., M. Dekker, New York, (1998); Ch. 18, pp. 417-435.

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

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

Invited Lectures

72nd ACS Colloid and Surface Science Symposium, The Pennsylvania State University, June 1998, "Dynamic Surface Tension of Aqueous Lung Surfactants: A Comparison of Practical Systems to Model Systems," with S.Y. Park and R.E. Hannemann.

Meeting Presentations

AIChE Annual Meeting, Los Angeles, California, Presentations November 1997, "Unusually Low Dynamic Surface Tensions Under Pulsating Area with Solutions of Ionic Surfactant," with X. Wen and K.A. Coltharp.

AIChE Annual Meeting, Los Angeles, California, November 1997, Effects of Chain Length and Dispersed Particles on Dynamic Surface Tension of Alcohols;" with S.H. Myrick, presented by S.M. Myrick.

NOBCCHE (National Organization of Black Chemists and Chemical Engineers), Dallas, Texas, April 1998, "Effect of Chain Length on Equilibrium and Dynamic Surface Tension of Spread Monolayers of Aqueous Alcohols;" S.M. Myrick and E.I. Franses, presented by S.M. Myrick.

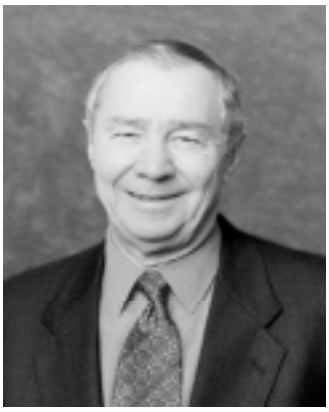
Surfactant Workshop, Aguadulce, Spain, June 1998, "Aggregation Properties of bis(Args) Gemini Surfactants in Aqueous Media," with A. Pinazo, L. Perez, X. Wen, E.I. Franses, and M.R. Infante, presented by A. Pinazo.

Robert A. Greenkorn

1965

R. Games Slayter Distinguished Professor of Chemical Engineering

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



Degrees

BS, University of Wisconsin, 1954

MS, University of Wisconsin, 1955

PhD, University of Wisconsin, 1957

Interests

Flow phenomena in porous media

Pollution prevention

System modeling

Awards and Major Appointments

Editorial Board, *Transport in Porous Media*

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

Member of the University Corporation for Atmospheric Research (UCAR)

Research Coordinator for the Clean Manufacturing and Safe Materials Institute

Director, Purdue Technical Assistance Program

Research Areas

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

Pollution Prevention: The clean Air Act of 1990 requires regulation of emissions of hazardous air pollutants (HAP). The Environmental Pro-

tection Agency has issued proposed regulations (1) to reduce emissions of toxic air pollutants from the flexible polyurethane foam industry. These National Emissions Standards for Hazardous Air Pollutants (NESHAP) apply to manufacturers of slabstock foam, molded foam and rebond foam. Similar legislation exists in Germany. The major pollutant in question is methylene chloride, which is used in the foam industry as a solvent, a cleaning liquid and a blowing agent. To use cleaner industrial processes and prevent emission of low boiling solvents such as methylene chloride, the Indiana Clean Manufacturing and Safe Materials Institute and the Research Group on the recycling of plastics at the Technische Fachlochschule Wildau are cooperating to evaluate processes and techniques proposed to mitigate the emissions problem.

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

Publications

Greenkorn, R.A., Kuo, R. Keith and Cushman, J.H., Experiments to verify Non-Local Dispersion theory in Aperiodic Heterogeneous Porous Media, "*AIH Advances in Ground-water Hydrology*, Ed. Walker, K.M. and Zaporozec, A. p 306 (1997).

Irwin, N.C., Altobelli, S.A., Cushman, J.C. and Greenkorn, R.A., "NMR Imaging Experiments for the Verification of Stochastic Transport Theory," *Magnetic Resonance Imaging*, In press (1998).

Meeting Presentations

Irwin, N.C., Altobelli, S.A. and Greenkorn, R.A. (Speaker). "Experimental Verification of Theory for Dispersion by NMR Imaging in Heterogeneous Porous Media," Fourth International Meeting on Recent Advances in NMR Applications to Porous Media, Trondheim, Norway, Aug. 31 - Sept. 3, 1997.

Greenkorn, R.A. (Speaker), Kuo, R. Keith and Cushman, J.H., "Experiments to verify Non-Local Dispersion Theory in Aperiodic Heterogeneous Porous Media," International Conference on Advances in Ground-Water Hydrology, American Institute of Hydrology, Tampa, FL, Nov 16-20, 1997, invited.

Robert E. Hannemann

1969

Visiting Professor

Degrees

BSCHE, Purdue University, 1952

MD, Indiana University, 1959

Interests

Engineering in medical research and practice

Aerosols in medical practice

Surfactants in respiratory distress syndrome treatment

Non-invasive diagnostic techniques

Serum bilirubin determination by skin reflectance

Awards and Major Appointments

Pediatrics *Editorial Board*

Secretary's (Health and Human Services) Advisory Committee on Infant Mortality

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 SpectR_x 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 Saturated Drying," with Achanta, S., M. Okos and J. Cushman, *AIChE J, Vol. 43, No. 8*, p. 2112ff, (August 1997).

Momentum, Heat, and Mass Transfer Fundamentals, with R. A. Greenkorn, to be published by Marcel Dekker, Inc.

Hilary S. Lackritz

1991

Adjunct 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

Jochen A. Lauterbach

1996

Assistant Professor

Degrees

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

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

Interests

Surface chemistry and heterogeneous catalysis

Laser light based microscopy and spectroscopy

Time-resolved IR vibrational spectroscopy

Non-linear phenomena in catalysis

Low temperature oxidation catalysts

Polymer - metal interfaces

Combinatorial catalysis

Awards and Major Appointments

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

Research Areas

Many chemical processes involving surfaces, such as heterogeneously catalyzed reactions, semiconductor etching, or coating can be spatially inhomogeneous. This fact, however, is often neglected simply because no suitable microscopic tools are available to follow those processes in situ. To gain full understanding and control of the temporal and spatial dynamics, it is mandatory to employ both spectroscopy and microscopy techniques, preferably simultaneously.

The long-term objective of our research is to study problems in heterogeneous catalysis and photopolymerization onto metal surfaces using novel surface imaging methods based on ellipsometry. Those techniques are combined with traditional vibrational and non-linear optics spectroscopy methods to perform in situ experiments in the following two research areas.

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

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

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

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

Publications

S. Lau, J. Right, K. Stavens, J. Whitaker, Z. Liu, and J. Lauterbach, “Do-It-Yourself Attenuated Total Reflectance Cell Designed and

Constructed in a Laboratory Course: A Versatile and Economical Alternative to Commercial Designs," *The Chemical Educator, 2(4), (1997).*

J. Lauterbach, S. White, X. Lui, G. M. Bodner, and W.N. Delgass, "A Novel Laboratory Course on Advanced Chemical Engineering Experiments," *Chemical Engineering Education, 31(4)*; 260-265, (1997).

M. Sushchikh, J. Lauterbach, and W.H. Weinberg, "Adsorption and Desorption Kinetics of CO on Ir(111): Bridging the Pressure Gap," *Surface Science, 393*, 135-140, (1997).

G. Haas, T.D. Pletcher, G. Bonilla, T.A. Jachimowski, H.H. Rotermund, and J. Lauterbach, "Ellipsomicroscopy for Surface Imaging - A Novel Tool to Investigate Surface Dynamics," *Journal of Vacuum Science and Technology A, 16(3)* 1117-1121, (1998).

Invited Lectures

J. Lauterbach, "Ellipsomicroscopy for Surface Imaging-A Novel Tool to Investigate Surface Dynamics," presented at the physics seminar of FORD Scientific Lab, FORD Motor Company, Dearborn, MI, September 1997.

J. Lauterbach, "Non-linear phenomena in surface reactions," presented at the Catalysis and Surface Science Center, Northwestern University, October 1997.

J. Lauterbach, "Imaging non-linear phenomena in surface reactions: the CO oxidation on platinum," presented at the Physics Department, University of Bayreuth Germany, July 1998.

Meeting Presentations

T. D. Pletcher, G. Haas, T. Jachimowski, and J. Lauterbach, "Unsteady behavior of CO and propylene oxidation on model platinum catalysts: Transition from isothermal to non-isothermal reaction regime," presented at the fall meeting of the American Chemical Society, Las Vegas, NV, September 1997.

J. Lauterbach, S. White, G. M. Bodner, X. Liu, and W. N. Delgass, "Advanced laboratory course for undergraduate and graduate students in chemical engineering and chemistry," presented at the workshop "Innovations in Laboratory Instruction," fall meeting of the American Chemical Society, Las Vegas, NV, September 1997.

G. Haas, T.D. Pletcher, G. Bonilla, T. A. Jachimowski, H.H. Rotermund, and J. Lauterbach, "Ellipsomicroscopy for Surface Imaging - A Novel Tool to Investigate Surface Dynamics," presented at the fall meeting of the American Vacuum Society, San Jose, CA, October 1997.

M. Sushchikh, J. Lauterbach, M. Schick, and W.H. Weinberg, "Adsorption of CO2 on the K-modified Ir(111) surface," presented at the fall meeting of the American Vacuum Society, San Jose, CA, October 1997.

J. Lauterbach, S. White, Z. Liu, G. M. Bodner, and W. N. Delgass, "Advanced ChE Lab Course for Undergraduate / Graduate Students," presented at the "Free Forum on Engineering Education," Fall meeting of AIChE, Los Angeles, CA, November 1997.

G. Bonilla, T.D. Pletcher, K.E. Green, G. Haas, T.A. Jachimowski, and J. Lauterbach, "Unsteady behavior of CO oxidation on platinum single crystals and supported catalysts - bridging the pressure gap," presented

at the Spring meeting of the American Physical Society, Los Angeles, CA, March 1998.

K.E. Green, T.A. Jachimowski, and J. Lauterbach, "A study of photopolymerization mechanisms on transition metal surfaces using time-resolved FT-IRAS," presented at the spring meeting of the American Physical Society, Los Angeles, CA, March 1998.

J. Right, G. Bonilla, T.D. Pletcher, and J. Lauterbach, "Unsteady Behavior of CO Oxidation on Platinum Single Crystals and Supported Catalysts," won 1st place at the Technical Paper Competition of the North Central Regionals of AIChE, Urbana, IL, March 1998.

G. Bonilla, T.D, Pletcher, G. Haas, and J. Lauterbach, "Unsteady Behavior of CO oxidation over Pt catalysts: Self-sustained Rate Oscillations in the Torr Pressure Range," presented at the Chicago Catalysis Club, Chicago, IL, May 1998.

G. Bonilla, T.D, Pletcher, G. Haas, and J. Lauterbach, "Unsteady Behavior of CO oxidation over Supported Pt catalysts and Pt single Crystals: Self-sustained Rate Oscillations in the Torr Pressure Range," presented at the 3rd International Conference on Unsteady-state Processes in Catalysis, St. Petersburg, Russia, June 1998.

Joseph F. Pekny

1990

Associate Professor

Degrees

BS, Princeton University, 1985

PhD, Carnegie-Mellon University, 1989

Interests

Process scheduling, planning, & design

Risk Management

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 to quickly solve the large scale optimization problems implied by the complex nature of integrated industrial processes. Thus, developing algorithms for highly structured and large scale manufacturing optimization problems is a research challenge involving the interaction of process physics, computer science, and applied mathematics. The goal is to engineer algorithms which provide high quality answers using

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

Our research over the last several years has shown that the formalism of mixed integer linear programming (MILP) based models offers a unique combination of scalability and flexibility—the ability to extract answers of provable quality and the potential for significantly lower installation and maintenance costs relative to other modeling technologies. Within the MILP domain a number of research areas are critical to achieving more capable optimization algorithms. In particular, twentieth century mathematics has disproved the notion of generic solution algorithms that can capably address all 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, parametric optimization, and risk analysis. A major goal of this research is° the ability to dynamically answer questions such as the following: how much inventory or idle capacity should be kept as an insurance policy, when should an order be promised for

delivery to a customer, is external (third-party) 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. An important practical outcome of the proposed research will be quantitative and qualitative methods for making the risk and reward of options more intuitive and provide details as to the potential impact of uncertainty and how it propagates through manufacturing networks.

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

Publications

P. Dave, D. Willig, G. Kudva, J. Pekny, and F. Doyle, "Linear Programming Methods in the Model Predictive Control of Large Scale Systems - An Application to the Cross Direction Control of a Paper Machine," *AIChE Journal, 43, No. 4,* pp. 1016-1031, (1997).

R. Ramakrishnan, B. Ramachandran, and J.F. Pekny, "A Dynamic Monte Carlo Algorithm for Exploration of Dense Conformational Spaces in Heteropolymers," *J. Chem. Phys.,1 06, No. 6,* pp. 2418-2425, (1997).

R. M. Wajge, J. M. Wilson, J. F. Pekny, and G.V. Reklaitis, "Investigation of Numerical Solution Approaches to Multicomponent Batch Distillation in Packed Beds," *Ind & Eng Chem Res, 36, No. 5,* p. 1738-1746, (1997).

M. H. Bassett, J. F. Pekny, and G. V. Reklaitis, "Using Detailed Scheduling to Obtain Realistic Operating Policies for a Batch Processing Facility," *Ind & Eng Chem Res, Vol. 36, No. 5,* pp. 1717-1726, (1997).

G. V. Reklaitis, J. Pekny, and G. S. Joglekar, "Scheduling and Simulation of Batch Processes," *Handbook of Batch Process Design*, pp. 24-60, Blackie Academic & Professional, an imprint of Chapman & Hill, London, (1997).

G. Applequist, O. Samikoglu, J. Pekny, and G. Reklaitis, "Issues in the Use, Design, and Evolution of Process Scheduling and Planning Systems," *ISA Transactions, 36,* , 81-121, (1997).

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

Meeting Presentations

J. Pekny, G. Kudva, S. Subrahmanyam, and M. Zentner, "Modeling, Algorithm, and Decision Tool Architecture Issues Associated With Process Industry Supply Chain Problems," Spring National Meeting, Houston, TX, session 104, 1997.

M. H. Bassett , J. F. Pekny, and G. V. Reklaitis, "Obtaining Realistic Production Plans for Batch Production Facilities," ESCAPE-7 / PSE 97, Trondheim, Norway, 1997.

F. J. Doyle, J. F. Pekny, G. V. Reklaitis and V. Venkatasubramanian, "A Graduate Course in Computer Integrated Process Operations," ESCAPE-7 / PSE 97, Trondheim, Norway, 1997.

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Nicholas A. Peppas

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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

Whitaker Best Paper Award, International Society for Artificial Organs, 1997

Fellow, American Institute of Chemical Engineers, 1997

Research Areas

Diffusion in and Dissolution of Glassy Polymers: Penetrant transport in glassy polymers may be described by two coupled processes of penetrant diffusion and macromolecular relaxation. Dissolution of glassy polymers can be considered as a combination of solvent penetration featuring Case II transport and polymer dissolution controlled by polymer disentanglement. Anomalous transport models are developed for solvent penetration which is coupled with a disentanglement model for polymer dissolution. Solvent penetration is controlled by the relaxation or deformation of polymer and the diffusional Deborah number is shown to be a major model parameter. In the disentanglement model, dissolution of polymer molecules requires that solvent concentration be greater than a critical gel concentration and that a polymer molecule be allowed a certain time to complete the disentanglement or diffusion movement from the gel state to liquid state. This time is assumed to be equivalent to the reptation time, which is a function of molecular weight, solvent concentration and chain rigidity. A concept of disentanglement clock is introduced as the material time clock controlling the dissolution. The new model may explain many experimental observations, such as effects of type of solvent and polymer on dissolution rate and the thickness of the gel layer. Experimental studies are performed with well-characterized samples of polystyrene and poly(methyl methacrylate) in various solvents using laser interfer-

ometer 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.

Structure, Morphology and Diffusive Properties of Heat-treated Poly(vinyl alcohol): When dilute, aqueous PVA solutions are cooled to -20 °C and thawed back to room temperature several times, a three dimensional network structure is formed due to the formation of relatively stable PVA crystals. This stable structure is further reinforced by an increased number of freezing / thawing cycles. PVA gels membranes / films / hydrogels made by this process are very desirable for a wide range of applications because they are free of toxic materials.

We are investigating the network structure and crystal size distribution in these gels. Using dynamic and equilibrium swelling studies, X-ray diffraction, differential scanning calorimetry, and ATR- FTIR spectrophotometry we analyze the crystal size and size distribution, the degree of crystallinity, etc. Stress-relaxation experiments is used to study the mechanical behavior of such systems and analyze the elastic behavior.

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

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

Highly Crosslinked Poly(Meth)Acrylates for Information Storage Materials: The kinetics of polymerizations of multifunctional acrylate and methacrylate monomers as well as the crosslinked structure and properties of the ensuing polymers are studied by a variety of experi-

mental techniques. Interferometric studies are used to calculate the relaxation of the polymer during the reaction, whereas shrinkage studies are related to conversion and the structure of the reacting monomers. The mesh size of the produced networks is analyzed using swelling studies. Differential scanning calorimetry and related thermal techniques provide information about this structure and mechanical properties of these networks. The results are used to verify and improve a kinetic model based on relaxation and to study relationships between monomer structure and applications in the information storage field.

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

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

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

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

homopolymers based upon complexation, hydrophobic interactions, and ionization equilibrium.

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

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

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

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

tailored for a variety of uses including catalysis of toxic molecules and molecular recognition, which have been demonstrated at sites covalently bonded to the interior architecture (molecular imprinting).

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

Drug and Protein Transport in and Interaction 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 drug release. An alternative release system based on interpenetrating polymeric networks of complexing is also developed. Finally, pH-sensitive hydrogels of poly(hydroxyethyl acrylic acid) are synthesized in the presence of water at concentrations larger than the equilibrium concentrations of the corresponding gels. When these systems are loaded with drugs or proteins and swollen in constant pH solutions, they deswell (collapse) transforming the polymer system into

a highly porous gel. Thus, the incorporated drugs can be released at constant rates. The release process is dependent on the pH and temperature of the solution. Experimental studies of drug release from such systems will be carried out and the overall release behavior will be modelled.

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

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

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

with the Hoshi University, Tokyo, Japan we conduct studies of nasal delivery of such systems.

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

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C.S. Brazel and N.A. Peppas, "Mechanisms of Solute and Drug Transport in Relaxing, Swellable, Hydrophilic Glassy Polymers," *Polymer* (in press).

M.T. am Ende and N.A. Peppas, "FTIR Spectroscopic Investigation and Modeling of Solute/Polymer Interaction in the Hydrated State," *J. Controlled Release*, (in press).

J. Siepmann, K. Podual, M. Sriwongjanya, N.A. Peppas and R. Bodmeier, "A New Model Describing the Swelling and Drug Release Kinetics from HPMC Tablets," *J. Pharm. Sci.*, (in press).

R.A. Scott and N.A. Peppas, "Kinetics of Copolymerization of PEG- (in press).

R.A. Scott and N.A. Peppas, "Compositional Effects on Network Structure of Highly Crosslinked Copolymers of PEG-Containing Multiacrylates with Acrylic Acid," *Macromolecules*, (in press).

R.A. Scott and N.A. Peppas, "Highly Crosslinked, PEG-Containing Copolymers for Sustained Solute Delivery," *Biomaterials*, (submitted).

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

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

Invited Lectures

"Poly(vinyl alcohol)-based Gels by Freezing/Thawing Processes," Hokkaido University, Division of Biological Sciences, Sapporo, Japan, July 10, 1997.

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

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

Chaired Conferences/ Symposia

Scientific Committee, Recent Advances in Drug Delivery Systems and Pharmaceutical Technology, June 1997.

Organizer and General Chairman of Topical Conference on "Biomaterials, Carriers for Drug Delivery and Scaffolds for Tissue Engineering," AIChE Meeting, Los Angeles, CA, November 1997.

Chairman of Session on "Drug Delivery," 4th US-Japan CRS Meeting, Kauai, HI, December 1997.

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

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

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

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

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

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

Meeting Presentations

"Design of Oral Controlled Drug Delivery Systems for Insulin," 11th World Congress of the International Society for Artificial Organs, Providence, RI, July 1, 1997 (A)*.

"Variable-rate Implantable Insulin Infusion Pumps: Closed-loop Maintenance of Normoglycemia Under Patient Variability for Type I Diabetes," 11th World Congress of the International Society for Artificial Organs, Providence, RI, July 1, 1997 (A)*.

"Poly(ethylene glycol)-Tethered Controlled Release Systems with Improved Mucoadhesive Behavior: Preparation and Studies with ATR-FTIR Spectroscopy," Japanese Drug Delivery Systems Society Meeting, Sapporo, Japan, July 11, 1997(P), Plenary Lecture.

"Biomaterials for Developing Pharmaceutical Preparations of High Quality of Life," Annual Meeting of Academy of Pharmaceutical Sciences and Technology, Kitamazu, Chiba, Japan, July 14, 1997 (P), Plenary Lecture.

"Protein Delivery from Novel Bioadhesive Complexation Hydrogels," Alfred Benzon Symposium, Copenhagen, Denmark, August 19, 1997 (A), Invited Lecture.

"Self-diffusion and Molecular Mobility in PVA-based Dissolution-Controlled Systems for Drug Delivery," Fourth International Meeting of Recent Advancesin Magnetic Resonance Applications to Porous Media, Trondheim, Norway, September 2, 1997 (A)*.

"Complexation Graft Copolymers as Oral Drug Delivery Systems," American Chemical Society Meeting, Las Vegas, NV, September 9, 1997 (P)*.

"Novel Copolymeric Acrylate Networks for Sustained Solute Delivery," American Chemical Society Meeting, Las Vegas, NV, September 10, 1997, (P)*.

"Preparation and Characterization of PEG-Containing pH-Sensitive, Cationic Hydrogels for Drug Delivery Applications," American Chemical Society Meeting, Las Vegas, NV, September 10, 1997, (P).

"Morphology of Poly(Vinyl Alcohol) Gels Prepared by a Freezing/Thawing Process," American Chemical Society Meeting, Las Vegas, NV, September 10, 1997, (A).

"Time and Frequency Domain Analysis of Blood Glucose Regulation Algorithms," 19th IEEE Engineering in Medicine and Biology Conference, Chicago, IL, November 1, 1997, (A)*.

"The Importance of the Drug Diffusion Front in Drug Delivery Kinetics from Swellable Matrices," American Association of Pharmaceutical Scientists Meeting, Boston, MA, November 4, 1997, (A)*

"Design of Oral Delivery Systems for Peptides and Proteins Using Complexation Graft Copolymer Networks," Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P)*.

"Molecular and Release Characteristics of Dissolution-Controlled Drug Delivery Systems," Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P)*.

”Glucose-Sensitive Cationic Hydrogels: Preparation Characterization and Modeling of Swelling Properties,” Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P)*.

“Analysis of Insulin Administration and Absorption from Ocular/Lacrimal/Nasal Systems with or without Enhancers,” Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P)*.

“Control Analysis of Pancreas Models for Optimal Insulin Delivery,” Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P)*.

“Protein and Drug Transport in PVA/PAA Composite Membranes Prepared by Freezing/Thawing Techniques,” Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P).

“Probing the Network Structure of Highly Crosslinked Ionizable Polymers,” Annual Physical Society Meeting, Los Angeles, CA, March 18, 1998, (A)*.

“Network Structure and Diffusion in Highly Crosslinked Ionizable Polymers,” Annual Physical Society Meeting, Los Angeles, CA, March 18, 1998, (A)*.

“NMR Imaging Analysis of Self-Diffusion and Molecular Mobility During Dissolution of Water-Soluble Polymers,” Annual Physical Society Meeting, Los Angeles, CA, March 18, 1998, (A)*.

“Protein and Drug Transport in PVA/PAA Composite Membranes Prepared by Freezing/Thawing Techniques,” Annual AIChE Meeting, Los Angeles, CA, November 18, 1997, (P).

“Physicochemical and Mathematical Factors Influencing Drug Delivery,” Annual Society for Biomaterials Meeting, San Diego, CA, April 21, 1998, (A), Invited Lecture.

“Novel Bioadhesive Complexation Gels for Oral Peptide Delivery,” Annual Society for Biomaterials Meeting, San Diego, CA, April 23, 1998, (P)*.

“Polymer Relaxation in Swellable Matrices Contributes to Drug Release,” 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

“Pure PVA Hydrogels Using Freezing/Thawing Techniques as Carriers for Drug Delivery,” 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

“Insulin Release from pH-Sensitive Cationic Hydrogels,” 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

“Molecular Design of Ionizable PEG-Containing Networks for Extended Solute Release,” 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

“Drug Transport Analysis in Complex Networks Using Molecular Probes,” 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

"Modelling of Controlled Release Systems for Consumer Products," 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

"Synthesis and Characterization of Poly(ethylene glycol) Star Polymer Gels for Medical and Pharmaceutical Applications," 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

"Novel PNIPAAm / PMAA Interpenetrating Polymer Networks," 25th International Symposium on Controlled Release of Bioactive Materials, Las Vegas, Nevada, June 22, 1998, (P).

Doraiswami Ramkrishna

1976

Harry Creighton Peffer Distinguished Professor of Chemical Engineering

Degrees

BS, University of Bombay, 1960

PhD, University of Minnesota, 1965

Interests

Chemical reaction engineering

Dispersed phase systems

Biochemical engineering

Applied mathematics

Awards and Major Appointments

AIChE Richard Wilhelm Award in Chemical Reaction Engineering, 1998

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

Research Areas

Chemical Reaction Engineering: Research emphasis in reaction engineering is on orchestration of interfacial mixing and reaction to promote selectivity and conversion in heterogeneous reactors. In collaboration with Professor Delgass, the investigation of spatial patterns has shifted towards mixing catalysts in order to feature auxiliary reactions that "correct" unfavorable trends in the main reaction system. Catalyst mixing is considered from the intra pellet scale using composite pellets, to the pellet scale of mixing different pellets, and on to the reactor scale comprising layered spatial patterns of different beds with suitably varying reaction conditions. Preliminary calculations show that such patterns have the potential to vastly improve reactor operation in terms of conversion and selectivity. Analysis of the stability and sensitivity of patterns is under way with focus on the effects of pattern breaking perturbations. Applications to several commercially significant reaction systems are under investigation.

Dispersed Phase Systems: A procedure for the inversion of dynamic particle size distributions to calculate nucleation and growth kinetics of crystallization and precipitation systems has been developed recently in our group. The advantage of this procedure lies in the identification of population balance models essential for controlling particle size in crystallization or precipitation processes even when models of theoretical origin are not available for nucleation and particle growth and may be

of special significance to complex biological systems. With Professor Doyle of the University of Delaware, the development of algorithms for control of particle size distributions in precipitation processes is in progress.

A new approach to hindered creaming of droplets based on a combination of population balance and experimental measurement of drop population densities has been developed for accurate measurement of creaming velocities of droplets in very dense polydisperse emulsions for which correlations have not been available in the past. Furthermore, well known hydrodynamic corrections to terminal velocities in denser dispersions appear to be in discord with experimental data obtained by this new technique. Simulation of the dynamics of creaming of polydisperse emulsions show the variation in the structure of the cream layer as the initial conditions of the emulsion are varied. Coalescence of droplets in the cream layer is also being initiated in the project towards the goal of determining shelf-life.

Other activities include population balance modeling of particle size distributions in precipitation and crystallization processes particularly in small systems such as emulsion droplets, reverse micelles etc. 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.

Biochemical Engineering: Nonlinear mathematical analysis of cybernetic models has revealed the full multiplicity and stability structure which govern microbial response to complex media. 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.

Cybernetic modeling concepts have been applied to problems in metabolic engineering with successful applications to numerous case studies established in the literature.

Nonlinear analysis of cybernetic models for continuous bioreactors to elucidate steady state multiplicity and Hopf bifurcation behaviors are in progress. Cybernetic models for hybridoma cell reactors predict state multiplicity observed in the experiments of Hu and coworkers at the University of Minnesota.

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 Basaran, we are involved in an investigation of break-up of liquid droplets exposed to a random pressure field characteristic of turbulent flow.

Publications

Narang, A., A.E. Konopka and D. Ramkrishna, "New Patterns of Mixed Substrate Utilization During Batch Growth of Escherichia coli," *Biotech & Bioeng*, *55*, 747-757, (1997).

Narang, A., A.E. Konopka and D. Ramkrishna, "The Dynamics of Microbial Growth in Mixtures of Substrates in Batch Reactors," *J. of Theoretical Biology, 184*, 301-317, (1997).

Narang, A., A.E. Konopka and D. Ramkrishna, "Dynamic Analysis of the Cybernetic Model for Diauxic Growth," *Chem. Eng. Sci., 52*, 2567-2578, (1997).

Ramakrishna, R., A. E. Konopka, and D. Ramkrishna, "Microbial Growth on Substitutable Substrates. Characterizing the Consumer Resource Relationship," *Biotech. & Bioeng., 54*, 77-90, (1997).

Trinh, S. and D. Ramkrishna, "Pattern Formation in Fixed Bed Catalytic Reactors - II. Pattern Classes," *Chem. Eng. Sci., 52*, 3561-3578, (1997).

Bandopadhyay, R., K. S. Gandhi, R. Kumar and D. Ramkrishna, "Modeling of Precipitation in Reverse Micellar Systems," *Langmuir, 13*, 3610-3620, (1997).

Krishnaswami, S., D. Ramkrishna and J. M. Caruthers, "Statistical-Mechanically Exact Simulation of Polymer Conformation in an External Field," *J. of Chem. Phys., 107*, 5929-5944, (1997).

Kumar, S. and D. Ramkrishna, "On the Solution of Population Balance Equations by Discretization-III. Nucleation, Growth and Aggregation of Particles," *Chem. Eng. Sci., 24*, 4659-4679, (1997).

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

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

Varner, J. and D. Ramkrishna, Metabolic Engineering From A Cybernetic Perspective: Aspartate Family of Amino Acids," *Metabolic Eng.*, (in press).

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

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

Varner, J. and D. Ramkrishna, "Metabolic Engineering from a Cybernetic Perspective-I. Theoretical Preliminaries," *Biotechnology Progress*, (submitted).

Varner, J. and D. Ramkrishna, "Metabolic Engineering From A Cybernetic Perspective II. Qualitative Investigation of Nodal Architectures and Their Response to Genetic Perturbation," *Biotechnology Progress*, (submitted).

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

Tobin, T. and D. Ramkrishna, "Modelling the Effect of Drop Charge on Coalescence in Turbulent Liquid-Liquid Dispersions," *Can. J. Chem. Eng.*, (Special Issue on Mixing), Eds. A. Nienow, (submitted).

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

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

Invited Lectures

Second Joint U.S. China Chemical Engineering Conference, May 19-22, 1997, Beijing, China. Keynote Lecture on "Cybernetic Modeling and Metabolic Engineering." (Lecture delivered by Professor G. T. Tsao in view of inability to attend the conference).

Department of Chemical Engineering, North Carolina A & T University, Greensboro, North Carolina, October 10, 1997. Lecture on "The Destabilization of Stored Emulsions."

Indian Institute of Chemical Engineers, Golden Jubilee Celebrations, December 15-18, 1997, New Delhi, India. Plenary Lecture XIII on "Destabilization of Stored Emulsions."

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

Meeting Presentations

Pirog, T., S. Kumar, G. Narsimhan and D. Ramkrishna, "Hindered Creaming Velocities in Polydisperse Emulsions. Experimental Results," Paper No. 90j, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

Kumar, S. and D. Ramkrishna, "Discretization Methods for Solution of Population Balance Equations of Processes with Aggregation, Nucleation and Growth," Paper No. 132e, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

Ramkrishna, D., S. Manjunath, K. S. Gandhi and R. Kumar, "Modeling of Precipitation in Small Systems," Paper No. 196b, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

Schell, J. and D. Ramkrishna, "On Self-Similarity of Microbial Populations," Paper No. 234f, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

Parker, R., F. Doyle and D. Ramkrishna, "Nonlinear Adaptive Horizon-based Predictive Control of a Bioreactor using a State Space Laguerre Model," Paper No. 235h, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

Varner, J. and D. Ramkrishna, "The Cybernetic Framework and Metabolic Engineering. Investigation of Amino Acid Production in Corynbacterium lactofermentum ATCC 21799," Paper No. 240f, A.I.Ch.E. Annual Meeting, 1997, Los Angeles, November 16-21, 1997.

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; Executive Committee 1997, Chair, International Committee, 1993-1997

Kirkpatrick Chemical Engineering Achievement Award, Board of Judges, 1991- , Chair, 1995-1997

Advisory Board, Department of Chemical Engineering, Carnegie-Mellon University, 1991-1997

Visiting Professor and External Examiner, Polytechnic University of Catalunia, Barcelona, Spain, July, 1997

External Examiner, Imperial College of Science, Technology, and Medicine, University of London, London, UK, January, 1998

Research Areas

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

Batch process design encompasses the selection of processing recipe, operational schedules, equipment number and sizes, plant layout, and the staging of plant expansions. Batch plant design problems are challenging because they involve discrete choices, dynamics, and parameter uncertainty. Their solution requires developments in process

and logistical decision modeling, combinatorial optimization techniques, combined discrete-continuous simulation methods, and probabilistic decision tools such as Monte Carlo methods. Problems of current interest include synthesis and design for waste minimization.

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

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

Publications

Bassett, M., J.F. Pekny, and G.V. Reklaitis, "Using Detailed Scheduling to Obtain Realistic Operating Policies for a Batch Processing Facility," *I&EC Research, 36, 1717-1726 (1997).*

Elkamel, A., M. Zentner, J.F. Pekny, and G.V. Reklaitis, "A Decomposition Heuristic for Scheduling the General Batch Chemical Plant," *Eng. Opt., 28,* 299-330 (1997).

Mockus, L. and G.V. Reklaitis, "Mathematical Programming Formulation for Scheduling of Batch Operations Based on Nonuniform Time Discretization," *Computers & Chem. Engr., 21,* No. 10, pp. 1147-1156 (1997).

Applequist, G., O. Samikoglu, J.F. Pekny, and G.V. Reklaitis, "Issues in the Use, Design, and Evolution of Process Scheduling and Planning Systems," *ISA Transactions, 36,* No. 2, pp. 81-121 (1997).

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

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

Elkamel, A., M. Zentner, J.F. Pekney, and G.V. Reklaitis, "A Decomposition Heuristic for Scheduling the General Batch Chemical Plant," *Eng. Opt*., 28, 299-330 (1997).

Wajge, R., J.M. Wilson, J.F. Pekny, and G.V. Reklaitis, "Investigation of Numerical Solution Approached to Multicomponent Batch Distillation in Packed Beds," *I&EC Research, 36*, 1738-1748 (1997).

Mockus, L. and G.V. Reklaitis, "A Bayesian Approach to Batch Process Scheduling," *Intl. Trans. Operational Research*, 4, pp. 55-65 (1997).

Androulakis, I.P. and G.V. Reklaitis, "Approaches to Asynchronous Decentralized Decision Making," *Computers & Chem. Engr*, (in press).

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

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

Chaired Confrences/ Symposia

International Perspectives: Models for Success, plenary session co-chair, CCR Annual Meeting, St. Louis, Sept., 1997.

Productivity Enhancement through Advanced Model-Based Technologies, session chair, ISA Tech 97, Anaheim, CA, Oct., 1997.

Batch Processing, session chair, European Symposium on Computer Aided Process Engineering - VIII, Brugge, Belgium, May, 1998,

Invited Lectures

"Practical Approaches to Planning / Scheduling under Uncertainty," Aspenworld 97, Boston, MA, Oct. 1997.

"Decomposition Strategies in Planning and Scheduling Problems in Batch Chemical Processing," Mitsubishi Chemical Company, Mini-symposium on Modeling and Optimization for Operation and Management in Chemical Plants, Santa Clara, CA, Dec, 1997.

"Recent Developments in Batch Process Scheduling," Department of Chemical Engineering, Massachusetts Institute of Technology, October, 1997. Also, Department of Chemical Engineering, University of California, Los Angeles, February, 1998

"Approaches to Uncertainty in Process Planning and Scheduling," Texas Distinguished Faculty Lecturer, Department of Chemical Engineering, University of Texas, Austin, April, 1998. Also, Department of Chemical Engineering, Ohio State University, May, 1998.

Meeting Presentations

"Scheduling a Serial Batch Line with Significant Process Uncertainty," paper 210b, AIChE Annual Meeting, Los Angeles, Nov., 1997.

"Robust Planning and Scheduling of Process Development Projects under Stochastic Conditions," paper 211a, AIChE Annual Meeting, Los Angeles, Nov., 1997.

"Industrial Applications of Robust Process Development Project Planning" paper 62d, AIChE National Meeting, New Orleans, March, 1998.

"Sensitivity Analysis for Project Planning and Scheduling under Uncertain Completions," European Symposium on Computer Aided Process Engineering - VIII, May, 1998, (see also *Computers & Chemical Engineering, 22S*, S871-S874, 1998).

"Multi-Level Strategies for Optimizing Campaign Structures for Reactive Batch Distillation Systems," 5th IFAC Symposium on Dynamics and Control of Process Systems, Corfu, Greece, June, 1998.

Eva Sevick-Muraca

1994

Associate Professor

Degrees

BS, University of Pittsburgh, 1983

MS, University of Pittsburgh, 1985

PhD, Carnegie Mellon University, 1989

Interests

Biomedical Optical Imaging and Spectroscopy

Optical Engineering

Inverse problems in optical engineering

Colloidal Science

Awards and Major Appointments

DuPont Young Faculty Award, 1996-1999

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

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

National Science Foundation Young Investigator Award, 1993 -1998.

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

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

National Institutes of Health Diagnostic Imaging and Radiology Study Panel Charter Member, Washington, DC, 1998-2001.

National Science Foundation Graduate Fellowship Review Panel, Washington, DC , February 1998.

Member of industrial research consortia:

Measurement and Control Engineering Center, University of Tennessee (Knoxville), National Science Foundation Industrial/University Cooperative Research Center, 1993 - 97. National Science Foundation I/UCRC for Industrial Pharmacy, Purdue University, 1995 - present.

Research Areas

The recent advances in laser diode technology and photodetection make possible the development of non-invasive sensors for biotechnology, clinical medicine, and process monitoring in the medical, chemical, and pharmaceutical industries. However, in these industries most real systems of interest multiply scatter light, making the extraction of important spectroscopic information difficult, if not impossible. One example in the biomedical domain is the propagation of near infrared light through several centimeters of tissue. Nearly everyone has observed the propagation of red light through his or her hand held near to a white light source. Near-infrared light is multiply scattered in tissues, enabling penetration into several centimeters of tissue depth, but disabling the simple determination of important tissue optical properties which could provide biochemical information of disease status. Another example lies in the process measurement arena. While 70-80% of the chemical based industry deals with particulate or dispersed phase process streams, there is virtually no feedback control for critical parameters of particle size distribution or volume fraction since multiple light scattering prevents on-line measurement of these parameters from traditional spectroscopic analysis.

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

Patents

"Fluorescence imaging system and measurement," E.M. Sevick-Muraca and D.Y. Paithankar, patent number: 08/702,060 (3/2/98).

"Analysis of particles with multiply scattered light," E.M. Sevick-Muraca, J. Pierce, H. Jiang, and J. Kao, application no.: 8/747,112 (filed 11/8/96).

Publications

Paithankar, D.Y. Chen, A.U., Pogue, B.W., Patterson, M.S., and E.M. Sevick-Muraca, "Imaging of fluorescent yield and lifetime from multiply scattered light re-emitted from tissues and other random media," *Appl. Optics, 36:2260-2272, 1997.*

Sevick-Muraca, E.M., Pierce, J., Jiang, H., and J. Kao, "Photon migration measurement of latex size distribution in concentrated suspensions," *AIChE J., 43*: 655-664, 1997.

Jiang, H., Pierce, J., Kao, J., and E.M. Sevick-Muraca, "Measurement of particle size distribution and volume fraction in concentrated suspensions

using photon migration techniques," *Appl. Optics, 36*: 3310-3318, 1997.Sevick-Muraca, E.M., Lopez, G., Troy, T.L., Reynolds, J.S., and C.L. Hutchinson, "Fluorescence and absorption contrast mechanisms for biomedical optical imaging using frequency-domain techniques," *Photochemistry and Photobiology, 66*: 55-64, 1997.

Sevick-Muraca, E.M., Heintzelman, D.L., Lee, J., Troy, T., and D.Y. Paithankar, "The role of higher order scattering in solutions to the forward and inverse optical imaging problems in random media," *Appl. Optics, 36*:9058-9067, 1997.

Reynolds, J.S., Toy, T.L., and E.M. Sevick-Muraca, "Multi-pixel techniques for frequency-domain photon migration imaging," *Biotechnology Progress, 13*:669-680, 1997.

Sevick-Muraca, Eva M., Jiang, H., Hutchinson, C.L., and D.Y. Paithankar, "Fluorescence lifetime spectroscopy and imaging in scattering media with frequency-domain techniques," in *Applications of Optical Engineering to the Study of Cellular Pathology*, Ed. Kohen, 1997.

Jiang, H., Pierce, J., Kao, J., and E.M. Sevick-Muraca, "Frequency-domain photon migration techniques for on-line measurement of particle size distribution and volume fraction in concentrated process streams," *Laser Diode and LED Applications, II*, Ed. K. Linden, Proc. Soc. Photo-Opt. Instrum. Eng., *3000*: 99-109, 1997.

Sevick-Muraca, E.M. and D.Y. Paithankar, "Imaging of fluorescent yield and lifetime from multiply scattered light re-emitted from random media," *Advances in Fluorescence Sensing Technology III*, Ed. Richard Thompson, Proc. Soc. Photo-Opt. Instrum. Eng., *2980*: 303-318, 1997.

Lopez, G., Troy, T.L., Reynolds, J.S., Hutchinson, C.L., and E.M. Sevick-Muraca, "Detection of fluorescent and light absorbing optical hetereogeneities in tissue-mimicking phantoms using frequency-domain techniques," *Advances in Fluorescence Sensing Technology III*, Ed. Richard Thompson, Proc. Soc. Photo-Opt. Instrum. Eng., *2980*: 519-529, 1997.

Reynolds, J.S., Troy, T.L., and E.M. Sevick-Muraca, "Multi-pixel imaging of interfering photon density waves," *Proc. Soc. Photo-Opt. Instrum. Eng., 2979*: 122-128, 1997.

Chen, A. and E.M. Sevick-Muraca, "On the use of phosphorescent and fluorescent dyes for lifetime-based imaging within tissues," *Proc. Soc. Photo-Opt. Instrum. Eng., 2979*: 129-138, 1997.

Troy, T.L., Reynolds, J.S., and E.M. Sevick-Muraca, "Photon migration imaging using multi-pixel measurements," *Proc. Soc. Photo-Opt. Instrum. Eng., 2979*: 111-121, 1997.

Sevick-Muraca, E.M., Pierce, J., Hutchinson, C.L., Jiang, H. and M. Khalili, "Measurement of particle size distribution and volume fraction from frequency-domain measurements of photon migration," *Proc. Soc. Photo-Opt. Instrum. Eng., 2979*: 533-549, 1997.

Richter, S.M., Shinde, R.R., Balgi, G.V., and E.M. Sevick-Muraca, "Particle sizing using frequency-domain photon migration imaging," Part. Part. Syst. Charact., 15, 9-18, 1998.

Shinde, R.R., Balgi, G.V., Richter, S.M., Banerjee, S., Reynolds, J.S., Pierce, J.E., and E.M. Sevick-Muraca, "Investigation of static structure factor in dense suspensions using multiply scattered light," submitted to Applied Optics 3/98.

Banerjee, S., Shinde, R., and E.M. Sevick-Muraca. "Probing Static Structure with Multiply Scattered Light," submitted to Journal of Colloid and Interface Science, 5/21.

Sevick-Muraca, E.M., Reynolds, J.S., Troy, T.L., Lopez, G., and D.Y. Paithankar, "Fluorescence lifetime spectroscopic imaging with measurements of photon migration," in Advances in Optical Biopsy and Optical Mammography, Ed. R.R. Alfano, New York Academy of Sciences, Vol. 838, pp. 46-57, 1998.

Troy, T.L., and E.M. Sevick-Muraca, "Fluorescence lifetime imaging and spectroscopy in random media," in Applied Fluorescence in Chemistry, Biology, and Medicine, Rettig, ed., Springer Verlag, 1998.

Troy, T.L., Reynolds, J.S., and E.M. Sevick-Muraca, "Reconstruction of fluorescence lifetime and quantum efficiency using frequency-domain photon migration measurements," Optical Society of America Proceedings in Biological Optical Spectroscopy and Diagnostics, Sevick, Izatt, and Ediger, Eds. 1998.

Reynolds. J.S., Troy, T.L., Waters, D.J., Cornell, K.K., and E.M. Sevick-Muraca, "Multi-pixel freqeuncy-domain photon migration imaging of a fluorescent contrast agent," Optical Society of America Proceedings in Biological Optical Spectroscopy and Diagnostics, Sevick, Izatt, and Ediger, Eds.1998

Invited Lectures

"Photon migration for particle sizing in the chemical and pharmaceutical industries," Advances in Optical Techniques for Medicine and Surgery, The Engineering Foundation, Snowbird, UT, July 13-18, 1997.

"Fluorescence lifetime imaging and spectroscopy in tissues and highly scattering media: theory, measurement, and validation," SpectRX, Inc., Norcross, GA, August 28, 1997.

"Fluorescence lifetime imaging and spectroscopy in random media and tissues," 5th International Conference on Methods and Applications of Fluorescence Spectroscopy, Humboldt University, Berlin, September 21-24, 1997.

"Biomedical optical imaging with measurements of photon migration," Department of Biological Sciences Graduate Research seminar, Purdue University, September 3, 1997.

"Measurements of frequency-domain photon migration for characterization of particle interactions, size distribution, and volume fraction in concentrated particulate suspensions" Physical Chemistry Department Graduate Research seminar, Purdue University, December 3, 1997.

"Photon Migration Imaging for Medicine," Department of Chemical Engineering and Materials Science Graduate Seminar, Wayne State University, Detroit, MI, February 6, 1998.

"Photon Migration Imaging using fluorescent contrast agents," Photomedicine Lecture, Oregon Medical Laser Center, Portland, OR May 28, 1998.

Meeting Presentations

Sevick-Muraca, E.M., Reynolds, J.S.*, Troy, T.L., Paithankar, D.Y., Lopez, G. and J. Lee, "Fluorescence lifetime imaging with measurements of photon migration: theory, simulation, and experiment," IEEE Annual Meeting, Chicago, November 1997 (invited).

Shinde, R.R., Balgi, G.V., and E.M. Sevick-Muraca, "Investigation of static structure factor of concentrated polystyrene dispersions using photon migration," Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 1997.

Richter, S.M., Pierce, J.E., Hutchinson, G., and E.M. Sevick-Muraca, "Photon migration for use in the on-line monitoring of particulate process streams," Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 1997.

Troy, T.L., Reynolds, J.S., and E.M. Sevick-Muraca, "Photon migration imaging using multi-pixel measurements," Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 1997.

Sevick-Muraca, E.M., Richter, S.M., Hutchinson, C.L., Jiang, H., and J. Pierce, "Submicron particle sizing through measurement of photon migration developed for on-line analysis," Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 1997.

Reynolds, J.S.*, Troy, T.L., and E.M. Sevick-Muraca, "Fluorescence lifetime imaging," Eastern Analytical Symposium, New Brunswick, NJ, November 1997 (invited).

Banerjee, S., Shinde, R., and E.M. Sevick-Muraca, "Monitoring particulate suspensions undergoing depletion flocculation using frequency-domain photon migration," 72nd Colloid and Surface Science Symposium, American Chemical Society, Pennsylvania State University, June 19-23,1998.

Richter, S., Shinde, R., Reynolds, J.S., and E.M. Sevick-Muraca, "Incorporation of structure factor into frequency-domain photon migration for particle sizing,"72nd Colloid and Surface Science Symposium, American Chemical Society, Pennsylvania State University, June 19-23, 1998.

Shinde, R., Banerjee, S., Balgi, G. and E.M. Sevick-Muraca, "Photon Migration: a novel method for monitoring particle interactions in concentrated suspensions," 72nd Colloid and Surface Science Symposium, American Chemical Society, Pennsylvania State University, June 19-23, 1998.

Chaired Conferences/ Symposia

"Novel quantitative tools and experimental techniques in bioengineering," American Institute of Chemical Engineers, Los Angeles, CA, November 1997.

Organizing Committee Member, National Academy of Engineering Frontiers of Engineering Symposium Fourth Annual Meeting, Irvine California, September 1998.

Chair of Optical Society of America Topical Meeting for Biomedical Optical Spectroscopy and Diagnostics, Orlando, FL, March 1998.

Session Chair, "Photon Migration Imaging and Spectroscopy," in Gordon Research Conference on Lasers in Medicine and Biology, Kimball Union Academy, Meriden, NH, June 1998.

Editorial Boards

Photochemistry and Photobiology (Associate Editor) 1995 -1999.

Journal of the Optical Society of America A, (Special Topics Co-Editor, 1997 special issue on diffusing photons).

Applied Optics (Special Topics Co-Editor, 1997 special issue on bio-medical optics).

Special Topics Co-Editor, Lasers in Medical Science, special issue on Non-invasive optical biodiagnostics, 1998.

Jennifer Lynn Sinclair

1997

Associate Professor

Degrees

BS, Purdue University, 1983
MA, Princeton University, 1985

PhD, Princeton University, 1989

Interests

Gas-solid flow

LDV measurements in fluid-solid systems

CFD multiphase code development

Awards and Major Appointments

US Representative for US-South Africa Collaboration in Particle Technology, 1997

Member of the Executive Committee of the Particle Technology Forum

Editorial Advisory Board, Powder Technology, 1997 -

Best Session Award, AIChE Annual Meeting, 1997

NSF-ERC Site Review Panel for University of Florida ERC in Particle Science & Technology

Research Areas

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

In order to treat flows in systems of practical size where the solids loading ratio (ratio of solids mass flux to gas mass flux) exceeds 1, particle flow models are constructed in the Eulerian framework. Professor Sinclair's research work to date has focused on the development of

such models for dilute and dense-phase gas-solid flows and these models have been incorporated into the commercial CFD package Fluent, Version 4.5.

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

By coupling the flow equations with thermal energy balances for the gas and particle-phases, Professor Sinclair and students have also shown how the observed complex heat transfer behavior in gas-solid systems is related to the hydrodynamic behavior. In gas-solid flow with heat transfer, the Reynolds analogy is applied to both the gas and solid-phases. The dilute-phase flow, the heat transfer coefficient increases with increasing Reynolds number and decreasing particle size at a fixed solid loading due to an increase in interphase heat transfer. The two-phase heat transfer coefficient can increase or decrease with solids loading for a given particle size based on the competition between gas turbulence modulation and the effect of particle-particle collisions. In dense-phase, gas-solid flow with heat transfer, the effective thermal conductivity of the particle phase is augmented by particle velocity fluctuations at the level of individual particles and clusters of particles. The heat transfer coefficient in dense phase flow increases with increasing solids flux and/or decreasing superficial gas velocity due to an increase in the effective thermal conductivity of the particle phase. The heat transfer coefficient is also highly dependent on the solid segregation patterns and the solids volume fraction at the wall.

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

modeled using a kinetic theory treatment applicable to bimodal mixtures. Preliminary predictions reveal a reduction in particle phase stress in the bimodal mixture as compared to a monosized particle system with the same mean particle diameter.

Publications

C.M. Hrenya and J.L. Sinclair, "On the Effects of Particle Phase Turbulence in Dense Gas-Solids Flow," *AIChE J.* (1997) *43*, 853-869.

P. Agarwal and J.L. Sinclair, "The Role of Fines in the Transport of Gas-Solid Suspensions," Gas-Solid Flows, *ASME-FED* (1997) *245*, 1 - 8.

P. Agarwal and J.L. Sinclair, "The Effect of PSD in the Flow of Fluidized, Gas-Solid Mixtures," Proceedings of the Fluidization, Fluid-Particle Sessions, 1997 Annual AIChE Meeting, Los Angeles, CA (1997) 26-30.

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

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

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

Chaired conferences/ Symposia

Chair, Undergraduate Education in Particle Technology, 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.

Co-Chair, Turbulent Flow, 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.

Member, AIChE National Fluid Mechanics Programming Committee, 1996 - Present.

Scientific Committee, Fluidization IX, Durango, CO, May 1998.

Invited Lectures

"Case Studies: CFD in Multiphase Flows Involving Particles," 1997 ASEE Summer School, Snowbird, UT, August 1997.

"Latest Developments in the Modeling of Gas-Solid Flows," DuPont Company, Wilmington, DE, October 1997.

"Modeling the Flow Behavior of Gas-Particle Suspension," Inhale Therapeutic Systems, Palo Alto, CA, October 1997.

"Dilute and Dense-Phase Gas-Solid Flow," University of Washington, Department of Chemical Engineering, Seattle, WA, January 1998.

"Gas-Solid Flow Simulation," National Science Foundation Workshop on Flow of Particulates and Fluids, Santa Barbara, California, February 1998.

"Modeling and Measurement of Dilute and Dense-Phase Gas-Solid Flows," Princeton University, Symposium Honoring the Retirement of Professor Roy Jackson, Princeton, NJ, April 1998

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

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

Meeting Presentations

"Particle-Turbulence Interaction," 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.

"The Effect of PSD in the Flow of Fluidized, Gas-Solid Mixtures," 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.

"Modeling Heat Transfer in Dense-Phase Gas-Solid Flow," 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.

"The Role of Particle Size Distribution in the Pneumatic Conveying of Solids," Fluidization IX, Durango, CO, May 1998.

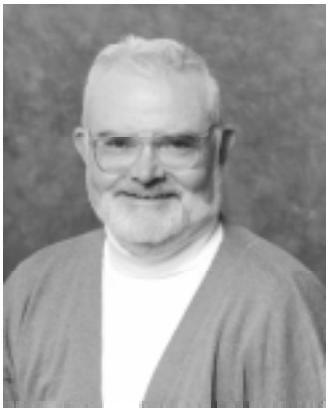
"Describing Particle-Turbulence Interaction in a Two-Fluid Framework," 1998 ASME Fluids Engineering Summer Meeting, Washington, DC, June 1998.

"CFD in Particle-Laden Flows," 1998 ASME Summer Meeting, Washington, DC, June 1998.

Robert G. Squires

1962

Professor



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

Interests Educational applications of computer simulation

George T. Tsao

1974

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

Degrees

BS, National Taiwan University, 1953

MS, University of Florida, 1956

PhD, University of Michigan, 1960

Interests

Biochemical Engineering

Renewable resource utilization

Biological Waste Conversion for Environmental Protection

Publications

Lark, N., Y. Xia, C.G. Qin, C.S. Gong, and G.T. Tsao, "Production of Ethanol from Recycled Paper Sludge Using Cellulase and a Thermotolerant Yeast, Kluveromyces marxianus," *Biomass and Energy 12*, 135-43 (1997).

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

Cao, N. J., C. S. Gong, and G. T. Tsao, "Production of Fumaric acid and L-Lactic Acid by Rhizopus and Their Applications." in *Recent Research Developments in Microbiology* (in press).

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

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

Du, J. X., N. J. Cao, C. S. Gong, and G. T. Tsao, "Effects of pH on Fumaric Acid Production in an Air-Lift Loop Reactor," *Applied Biochem. Biotechnol.* (in press).

Du, J. X., N. J. Cao, C. S. Gong and G. T. Tsao, "Production of L-Lactic Acid by Rhizopus oryzae in a Bubble Column Fermenter," *Applied Biochem. Biotechnol. 70-72,* 323-329 (1998).

Wang, X., C. S. Gong, and G. T. Tsao, "Production of L-Malic Acid via Biocatalysis Employing Wild type and Respiratory Deficient Yeasts." *Applied Biochem. Biotechnol. 70-72*. 845-852 (1998).

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Dominguez, J. M., C. S. Gong, and G. T. Tsao, "Production of Xylitol from D-Xylose by Debrayomyces hansenii," *Applied Biochem. Biotechnol. 63-65*, 117-127 (1997).

Krishnan, M. S., Y. Xia, N. W. Y. Ho, and T. T. Tsao, "Fuel Ethanol Production from Lignocellulosic Sugars: Studies Using a Genetically Engineered Saccharomyces Yeast," *ACS Symp. on Fuels and Chemicals from Biomass, Series no. 666*, 74-92 (1997).

Dominguez, J. M., N. J. Cao, M. S. Krishnan, C. S. Gong, and G. T. Tsao, "Xylitol Production from Hybrid Poplar Wood Chips Pretreated by Ammonia Steeping Process," *Biotechnol. Techniques 11*, 339-341 (1997).

Venkat Venkatasubramanian

1988

Professor

Degrees

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

MS, Physics, Vanderbilt University, 1979

PhD, Chemical Engineering, Cornell University, 1984

Interests

Process fault diagnosis and supervisory control

Process hazards analysis

Computer-aided molecular design and product formulation

Synthesis of operating procedures for batch process plants

Behavior of complex adaptive systems

Intelligent systems, neural networks, and genetic algorithms

Major Appointments

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

Member of the New Technology Task Force, American Institute of Chemical Engineers, 1996-98

Trustee, CACHE Corporation, 1996-99

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

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 annually 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 process 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 Lubrizol, Dow AgroSciences and Caterpillar corporations who are 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. It has been used in daily plant operations quite successfully since the beginning of 1998 by the industrial sponsor of this project. Current research integrating iTOPS with a process hazards analysis system.

Publications

R. Srinivasan, V. D. Dimitriadis, N. Shah and V. Venkatasubramanian, "Safety Verification Using a Hybrid Knowledge-Based Mathematical Programming Framework," *AIChE J*, *44(2)*, 361-371, (1998).

R. Srinivasan and V. Venkatasubramanian, "Automating HAZOP Analysis of Batch Chemical Plants: Part I. Knowledge Representation Framework," in press, *Computers and Chemical Engineering*, (1998).

R. Srinivasan and V. Venkatasubramanian, "Automating HAZOP Analysis of Batch Chemical Plants: Part II. Algorithms and Application," in press, *Computers and Chemical Engineering*, (1998).

S. Viswanathan, C. Johnson, R. Srinivasan, V. Venkatasubramanian, K-E. Arzen, "Automating Operating Procedure Synthesis for Batch Processes: Part I. Knowledge Representation and Planning Framework," in press, *Computers and Chemical Engineering*, (1998).

S. Viswanathan, C. Johnsson, R. Srinivasan, V. Venkatasubramanian, K-E. Arzen, "Automating Operating Procedure Synthesis for Batch Processes: Part II. Implementation and Application," in press, *Computers and Chemical Engineering*, (1998).

V. Venkatasubramanian and A. Sundaram, "Genetic Algorithms: Introduction and Applications," in the *Encyclopedia of Computational Chemistry*, John Wiley and Sons, (1997). (Invited book chapter)

S. R. McVey, J. F. Davis, and V. Venkatasubramanian, " Intelligent Systems in Process Operations, Design and Safety," *Computers in Chemical Engineering Education*, 25th Anniversary Issue, CACHE, Austin, Texas, (1997).

Meeting Presentations

R. Srinivasan and V. Venkatasubramanian, "PHAzer: An Intelligent System for Automated Process Hazards Analysis," in the Proceedings of International Conference of Risk Analysis in Process Safety, Atlanta, GA, Oct 21-24, 1997.

R. Srinivasan and V. Venkatasubramanian, "Multi-Perspective Models for Process Hazards Analysis of Large-Scale Chemical Processes," in the Proceedings of the European Symposium on Computer-Aided Process Engineering 8, Brugge, Belgium, May 1998.

H. Vedam and V. Venkatasubramanian, "A B-Spline Based Method for Data Compression, Process Monitoring and Diagnosis," in the Proceedings of the European Symposium on Computer-Aided Process Engineering 8, Brugge, Belgium, May 1998.

S. Viswanathan, L. Mockus, V. Venkatasubramanian, P. K. Basu, R. Mack, P. Cherukat, and V. Iskos, "iTOPS: An Intelligent Tool for Operating Procedure Synthesis," in the Proceedings of the European Symposium on Computer-Aided Process Engineering 8, Brugge, Belgium, May 1998.

H. Vedam and V. Venkatasubramanian, "Signed Digraphs for the Interpretation of PCA-based Fault Diagnosis," Proceedings of the IFAC International Conference on On-line Fault Detection and Supervision in the Chemical Process Industries, Lyon, France, June 4-5, 1998.

Invited Lectures

Intelligent Systems for Abnormal Situation Management, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, Oct 1997.

Recent Progress in Real-time Fault Diagnosis of Complex Chemical Plants, Exxon Chemicals, Baton Rouge, LA, Feb and May 1998.

Methodologies for Automating Plant Reference Model Development, Honeywell Technology Center, Minneapolis, MN, April 1998.

Intelligent Systems for Automated Process Hazards Analysis, Mary O'Connor Process Safety Symposium, Texas A&M University, College Station, TX, March 1998.

Abnormal Situation Management: Challenges and Opportunities, Department of Chemical Engineering, University of Texas, Austin, March 1998.

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 Batch Chromatography and Simulated Moving Bed Chromatography

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 concentrated aqueous solutions (1-14 M) of sodium hydroxide, sodium nitrite, and other electrolytes. We have developed 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. A case study of a

pilot carousel unit shows that 100% utilization of cesium capacity and maximum throughput can be achieved in an optimal design. Reducing sorbent particle size from 400 to 290 microns, for example, increases throughput by 40%. Our studies show that the simulations can significantly reduce the number of expensive and time-consuming experiments in process development. 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 Waste waters: Contamination of water supplies by synthetic organics, pesticides, herbicides, and other industrial chemicals is a widespread problem in the U.S. and many other countries. Many of the chemicals are known to be carcinogenic and must be removed to safeguard drinking water supplies and the environment. Among many treatment techniques, adsorption using activated carbon beds has been the best available technology for removing dissolved organics from a dilute (ppm level) solution. Because of high selectivity, activated carbon beds can achieve virtually complete removal of many organics. This technique, however, is quite expensive. Cost of treatment ranges from $0.1 to $19.00 per 1000 gal. This high cost is due to (1) process inefficiency as a result of low throughput and low capacity utilization, (2) high capital and labor costs due to the nature of batch operation in conventional technologies, (3) sorbent attrition and incomplete, costly regeneration, and (4) loss of the organics during sorbent regeneration. Research in our laboratory aims to find solutions to these key issues. We have recently developed a novel continuous separation process to recover amino acid derivatives and sodium chloride from a process stream containing 3.6 M sodium chloride and 40 mM of the amino acids. Preliminary results indicate that this process is a promising solution to an important industrial problem. The purity and recovery for the amino acid are 100% and 94% respectively. The cost of separation and recovery is estimated to be about $0.01 per gallon. We are seeking an industrial partner to license this technology, and to further develop this process for commercial applications. 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 process streams.

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, concentration, 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%). Ongoing research aims to improve the purity level and to further reduce the recovery and purification cost.

Simulated Moving Bed Chromatography for Biochemical Purification: In simulated moving bed chromatography, a series of columns containing a specific adsorbent are connected to form a circuit, which is divided

into four zones by two inlet (feed and desorbent) and two outlet (product and by-product) ports. The four ports are periodically moved along the fluid flow direction to allow the feed to enter the region where the solute bands overlap and the products to be drawn from the regions where the bands are separated. The periodic port movement simulates periodic counter current movement of the sorbent with respect to the ports, resulting in high sorbent utilization and high mass transfer rates. Since a major portion of the unseparated mixtures is automatically recycled within the circuit, SMB has much higher yield and lower desorbent consumption than corresponding batch chromatography processes. SMB, however, has not been widely used for large-scale biochemical purifications for the following reasons: (1) The SMB design is difficult, because it involves specifying a minimum of ten parameters (column diameter, four zone lengths, four flow rates, and an average port movement velocity). (2) Existing SMB's are designed for binary splits. How to design SMB's to separate multicomponent mixtures is not well known from the literature.

We have recently developed a standing wave analysis for continuous moving bed systems. For linear isotherm systems, simple algebraic equations are derived from the analysis to link product purity and recovery to zone lengths, bed movement velocity, flow rates, column capacity factors, and mass transfer coefficients. Once product purity and recovery are specified for a given system, the zone flow rates and recovery are specified for a given system, the zone flow rates and bed movement velocity that provide the highest throughput and the lowest solvent consumption can be determined from the solutions. The study shows that in a given system, there is a trade-off between product purity and throughput. Moreover, if bed volume and product purities are fixed, the longer the zone lengths, the higher the throughput. Dynamic simulations based on a detailed rate model that considers axial dispersion, film mass transfer, and intraparticle diffusion are developed and they are used to compare the column profiles and effluent histories of CMB and simulated moving bed (SMB). The comparison shows that the standing wave design equations derived for CMB systems are applicable to SMB systems. The extension of this analysis to nonlinear and multicomponent systems is in progress. This analysis has been used successfully in designing SMB systems for amino acid separations and sugar separations.

Publications

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.*, *43*, 232-242 (1997).

Ernest, M.V., Jr., R.D. Whitley, Z. Ma, and N.-H.L. Wang, "Effects of Mass Action Equilibria on Fixed-Bed Multicomponent Ion-Exchange Dynamics" *Ind. Eng. Chem. Res.*, *36*, pp. 212-226 (1997).

Ernest, M.V. Jr., J.P. Bibler, R.D. Whitley, and N.-H.L. Wang, "Development of a Carousel Ion Exchange Process for Removal of Cesium-137 from Alkaline Nuclear Waste," *Ind. Eng. Chem. Res., 36*, 2775-2788 (1997).

Ma, Z. and N.-H.L. Wang, "Standing Wave Analysis of Simulated Moving Bed Chromatography: Linear Systems," *AIChE J., 43(10),* 2488-2508 (1997).

Koh, J.-H., P.C. Wankat, and N.-H. L. Wang, "Pore and Surface Diffusion and Bulk-Phase Mass Transfer in Packed and Fluidized Beds," *I.E.C. Research, 37*, 228-239 (1997).

Ma, Z., and N.H.-L. Wang, "Designº of SMB Chromatography Using Standing Wave Analysis," 1997 AIChE Topical Conference on Separation Science and Technologies, Conference Proceedings. Paper No. 3265, 1010-1015 (1997).

Wu, D.-J., Y. Xie, Z. Ma, and N.-H.L. Wang, "Design and Optimization of SMB Chromatography for Separation of Two Amino Acids," 1997 AIChE Topical Conference on Separation Science and Technologies, Conference Proceedings, Paper No. 32h, 1455-1460 (1997).

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

Wu, D.J., Y. Xie, Z. Ma, and N.-H.L. Wang, "Design of SMB Chromatography for Amino Acid Separations," *I.E.C. Research*, in press.

Ma, Z., and N.-H. L. Wang, "Standing Wave Design of Nonlinear SMB Systems for Fructose Purification," *AIChE J.*, (accepted).

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

Jin, X., Z. Ma, J. Talbot, and N.-H.L. Wang, "A Model for the Adsorption Equilibria of Solutes with Multiple Adsorption Orientation," *Langmuir*, (accepted).

Meeting Presentations

D.J. Wu, Y. Xie, Z. Ma, and N.-H. L. Wang, "Design on Optimization of SMB Chromatography for Separation of Two Amino Acids," Symposium on Advances in Bioseparations-Adsorption and Chromatographic Separations, 1997 AIChE Annual Meeting, Chicago, IL. Nov. 16-21, 1997.

Z. Ma, and N.-H. L. Wang, "Design of SMB Chromatography Using Standing Wave Analysis," Symposium on the Fundamentals of Adsorption, 1997 AIChE Annual Meeting, Chicago, IL. Nov. 16-21, 1997.

D.J. Wu, R. D. Whitley, Z. Ma, and N.-H L. Wang, "Effects of Mass Transfer in Dynamic Nonlinear SMB Systems," the 6th International symposium on Fundamentals of Adsorption, Presquile de Giens, France, May 24-28, 1998.

Z. Ma, R. Wooley, and N.-H L. Wang, "Optimal Design of a Nine-zone SMB for Separations of Sugars from Acids in Biomass Hydrolysate," PREP 98, Washington D.C., May 31 - June 3, 1998.

K. Kauffman, Z. Ma, and N.-H. L. Wang, "Analysis, Dynamic Simulation, and Animation of SMB Chromatography for Large Scale Separation and Purification," PREP 98, Washington D.C., May 31-June 3, 1998.

Invited Lectures

"Continuous Adsorption Processes to Recover Amino Acid Derivatives and Salt from a Concentrated Salt Solution," Monsanto Company, St. Louis, MO, Nov. 11, 1997.

"Recovering and Purification of Clarithromycin from the Crystallization Mother Liquor," Abbott Laboratories, North Chicago, IL, Feb. 27, 1998.

"Batch Chromatography and Simulated Moving Bed Chromatography - Principles, Dynamic Simulations, and Design," Abbott Laboratories, North Chicago, IL, Feb. 27, 1998.

"Simulated Moving Bed Chromatography for Chemical and Biochemical Separations," Department of Chemical Engineering, University of Unicamp, Campinas, SP, Brazil, May 14, 1998.

"Simulated Moving Bed Chromatography for Chemical and Biochemical Separations," Department of Chemical Engineering, Federal University of Sao Carlos, SP, Brazil, May 15, 1998.

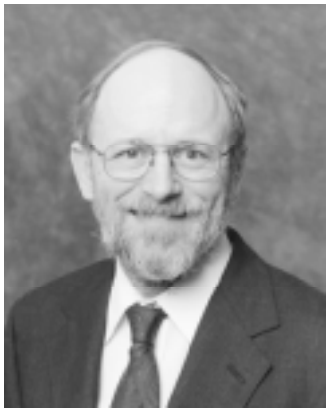
"Simulated Moving Bed Chromatography for Biochemical Separations-Design-Principles and Applications," Second Brazilian Adsorption Society Meeting, Florianopolis, Brazil, May 18-20, 1998.

"Analysis and Dynamic Simulation of Simulated Moving Bed Chromatography for Large Scale Separation and Purification," UOP, Des Plaines, IL. June 11, 1998.

Phillip C. Wankat

1970

Professor



Degrees

BS, Purdue University, 1966

PhD, Princeton University, 1970

MSEd, Purdue University, 1982

Interests

Adsorption and chromatography

Distillation

Teaching improvement

Awards and Major Appointments

Union Carbide Lectureship Award, Chem. Engr. Div., ASEE, 1997

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

Research Areas

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

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

Publications

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, 5-42 to 5-79 (1997).

Koh, J.-H., P.C. Wankat, N.-H.L. Wang, "Pore and Surface Diffusion and Bulk-Phase Mass Transfer in Packed and Fluidized Beds," *Ind. Engr. Chem. Res.*, *37*, 228-239 (1998).

Sundaram, N. and P. C. Wankat, "Dynamics of the Irreversible Michaelis-Mentin Kinetic Mechanism," *J. Phys. Chem.*, *102*, 717-721 (1998).

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

Arumugam, B.K., J. F. Banks and P. C. Wankat, "Pressure Effects in Adsorption Systems," Adsorption, (in press, 1998).

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

Wankat, P.C., "Synergism Between Research and Teaching Separations," invited ChE Division ASEE, Union Carbide Lectureship Award paper, *Chem. Engr. Educ., 31,* 202-209 (Fall 1997).

Hatton, D.M., P.C. Wankat and W.K. LeBold, "The Effects of an Orientation Course on the Attitudes of Freshman Engineering Students," J. *Engr. Educ., 87,* 23-27 (1998).

Wankat, P.C., "Engineering Education: Not Enough Education and not Enough Engineering," in S. Tornkvist (Ed.), *Proceedings Second International Conference on Teaching Science for Technology at Tertiary Level*, June 14-17, CD ROM ISBN 91-7170-219-9, (1997). Plenary Lecture

Wankat, P.C., "Educating Teachers," ASEE PRISM, 7 (8), 44 (April 1998). Invited paper for "Last Word" section of *PRISM*.

Wankat, P.C., "An Analysis of Articles in the Journal of Engineering Education," *J. Engr. Educ.*, (in press).

Editorial Boards

Separation and Purification Methods (Editor-in-Chief until 12/31/97; now on editorial board)

Chemical Engineering Education, Associate Editor

Separation Science and Technology

Adsorption

Chaired Conferences/ Symposia

Chair of Session, "Meet the Author," AIChE Meeting, Chicago, IL, November 1996 and AIChE Meeting, Los Angeles, CA, November 1997.

Co-Chair of Workshop, "Developing Problem Solving Skills," Steve LeBlanc (Chair), AIChE Meeting, Los Angeles, CA, November 1997.

Invited Lectures

"The Case of the Mysterious Adsorption Pressure," September 9, 1997, Chemical Engineering Department, West Virginia University, December 11, 1997, Chemical Engineering Department, University of Illinois-Chicago, and School of Chemical Engineering, Oklahoma State University, Stillwater, OK, February 19, 1998.
Organizer and Presenter, "Teaching Workshop for New Faculty," Chemical Engineering Division, ASEE Summer School, August 10, 1997, Snowbird, UT. [One-day workshop]
"Synergism Between Research and Teaching in Separations," Chemical Engineering Division, ASEE Union Carbide Lectureship Award, August 12, 1997, Snowbird, UT.

"Problem Solving in Engineering Education," Tis Lahiri Memorial Seminar, Department of Chemical Engineering, Vanderbilt University, Nashville, TN, October 26, 1997.

"Large-Scale Liquid Chromoatography," AspenWorld97, Boston, MA, October 14, 1997.

"Educating Engineering Educators in Engineering," Phillips Lecture, School of Chemical Engineering, Oklahoma State University, Stillwater, OK, February 20, 1998.

Projects Funded

Award Amount	PI/Sponsor/Title	Project Period
$440,389.00	R.P. Andres Army Research Office Electronic Conduction in Molecular Nanostructures	07/92-12/97
$450,000.00	R.P. Andres R. Reifenberger National Science Foundation Synthesis of Nanometer Diameter Particles and Measurement of Particle-Particle and Particle Substrate Interactions	05/92-07/98
$42,878.00	R.P. Andres Army Research Office Nanoelectronic Functional Devices: Architecture & Fabrication	09/96-02/98
$146,505.00	R.P. Andres Army Research Office Inst. For Chemical Sensing and Computational Applications of Molecularly Linked Networks of Nanometer Scale Metallic Clusters	03/98-03/99
$11,666.00	R.P. Andres Purdue Research Foundation Magnetic Thin Films	01/98-01/99
$10,000.00	O.A. Basaran Exxon Education Foundation Research into Micron-and-Sub-Micron Size Particle	10/94-09/97
$160,588.00	O.A. Basaran Dow Corning Corporation Computational Analysis of Fluid Mechanics of Distillation Trays	01/96-12/99
$280,000.00	O.A. Basaran NASA Forced Oscillations of Pendant and Sessile Drops	06/96-06/00
$327,033.00	O.A. Basaran DOE Fundamentals of Electric Field -Enhanced Multiphase Separations	08/96-08/99
$155,027.00	J.M. Caruthers AFOSR Fundamental Models for Predicting Lifetime Performance of High Performance Polymeric Materials	03/95-03/98
$11,666.00	J.M. Caruthers Purdue Research Foundation Study of Viscoelastic Relaxation During Chemical Deg Radiation in Polymer Solids	01/98-05/99

Award Amount	PI/Sponsor/Title	Project Period
$86,153.00	J.M. Caruthers Prairie View A&M Research Foundation Air Force Fast Center for Lightweight Structural Materials & Processing	09/95-09/98
$59,870.00	J.M. Caruthers Sandia National Laboratories Thermoviscoelastic Constitute Models for Engineering	09/97-09/98
$59,703.00	J.M. Caruthers Caterpillar, Inc. Application of Artificial Intelligence Methods for the Formulation of Engineering Plastics and Rubbers	07/98-07/99
$65,000.00	W.N. Delgass Dupont Central Research & Development Research for Expanding the Horizons and Overall Understanding of Heterogeneous Catalysis	12/94-09/99
$28,638.00	W.N. Delgass Purdue Research Foundation Dehydration of 2,3 Butanedial to Methyl Ethyl Ketone over Zeolite Catalysis	04/96-04/98
$18,323.00	W.N. Delgass E.I. Dupont de Nemours & Co. Promoted Fused Oxide Catalysts	05/97-05/98
$178,500.00	F.J. Doyle Office of Naval Research Neurobiologically Inspired Approaches to Nonlinear Process Control & Modeling	05/96-10/97
$167,122.00	F.J. Doyle National Science Foundation An Integrated Approach to Environmentally Conscious Paper Mill Operations	10/97-10/98
$28,638.00	E.I. Franses Purdue Research Foundation Effect of Processing Method on the Quality, Stability and Transport Properties of Thin Organic Films	04/96-04/98
$5,000.00	E.I. Franses Johnson & Sons Inc. Adsorption and Micellar Dynamics of Aqueous Surfactants	02/96-01/98
$191,920.00	E.I. Franses National Science Foundation Adsorption and Surface Tension of Surfactant/Lipid/Protein Mixtures: Direct Probing of Surface Layers and Theoretical Modeling	03/97-03/99

Award Amount	PI/Sponsor/Title	Project Period
$171,920.00	E.I. Franses (co-PI with T. Bein, C. Kubiak and P.Low) D. Ben-Amotz (PI) Purdue Research Foundation Development of a Chemical Imaging Microscope for Characterization of Micro-Composites and Biomaterials	06/97-05/98
$5,000.00	E.I. Franses Whirlpool Corporation Mass Transfer in Fabric Care	02/97-09\99
$50,881.00	R.A. Greenkorn Indiana Dept. of Environmental Management Indiana Pollution Prevention Institute	06/93-06/98
$42,874.00	R.A. Greenkorn Showalter Trust The Movement of Pollutants Underground	06/94-12/98
$27,423.00	R.A. Greenkorn Purdue Research Foundation NMR Imaging of Mixing During Flow in Heterogeneos Porous Media	07/96-07/98
$20,000.00	R.A. Greenkorn Peterson Charitable Foundation Peterson Technology Initiative	07/95-09/99
$500,000.00	H.S. Lackritz National Science Foundation NSF Presidential Faculty Fellows Program	08/93-07/98
$465,216.00	H.S. Lackritz Office of Naval Research High Temperatures Polymers for Second Order Nonlinear Optics: Photorefrative Polyimides for Photonic Materials	04/92-11/97
$93,569.00	H.S. Lackritz AFOSR Characterization of Optical Properties of Thin Nonlinear Optical Polymer Films for Device Applications as a Function of Processing	06/95-06/98
$20,000.00	J.A. Lauterbach American Chemical Society Non-linear Phenomena During Heterogeneously Catalyzed Reactions Observed with Ellipsomicroscopy	09/97-09/99
$5,000.00	J.A. Lauterbach Allied Signal, Inc. Phoenix Resource Center	09/96-09/99

Award Amount	PI/Sponsor/Title	Project Period
$70,603.00	J.A. Lauterbach National Science Foundation In Situ Microscopy and Spectroscopy of Dynamic Behavior	04/98-04/99
$399,000.00	J.F. Pekny National Science Foundation/Industry Presidential Young Investigator Award	08/90-09/99
$190,000.00	J.F. Pekny G.V. Reklaitis National Science Foundation A Comprehensive Approach to Chemical Process Scheduling Problems	04/94-08/98
$139,546.00	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	10/94-10/97
$40,000.00	J.F. Pekny Mobil Research & Development Corp. NSF-PYI Matching Funds	03/92-09/99
$28,892.00	J.F. Pekny Purdue Research Foundation Specialized Mathematical Programming Methods in the Model Predictive Control of Large Scale Systems	01/97-05/98
$10,972.00	N.A. Peppas NATO (N. Atlantic Treaty Organization) Investigation of Water and Solute Diffusion in Hydrophilic Polymers	03/94-01/98
$60,000.00	N.A. Peppas Showalter Trust Showalter Distinguished Professorship in Biomedical Engineering	11/93-06/98
$467,788.00	N.A. Peppas National Institute of Health PH Sensitive Complex Hydrogels and IPNS for Drug Release	09/95-09/98
$22,176.00	N.A. Peppas Purdue Research Foundation Glucose-Sensitive Systems for Insulin Delivery	01/96-01/98
$60,000.00	N.A. Peppas Showalter Trust Novel Mucoadhesive Biopolymers for the Targeted Delivery of Peptides and other Drugs to Tissue	07/96-07/99

Award Amount	PI/Sponsor/Title	Project Period
$363,636.00	N.A. Peppas National Science Foundation Polymer/Mucin Adhesion for Targeted Therapy	09/97-01/99
$163,339.00	N.A. Peppas National Institute of Health Peg-promoted Mucoadhesive Drug Delivery Systems	08/97-08/98
$29,000.00	N.A. Peppas Alcon Laboratories Polymerization Technologies	07/97-09/99
$25,400.00	N.A. Peppas Trask Trust Fund Method for Oral Delivery of Insulin	08/97-09/98
$315,000.00	F.J. Doyle + 250,000 (in kind) J.F. Pekny G.V. Reklaitis V. Venkatasubramanian Computer Integrated Process Operations Center Individually Supported	05/96-09/99
$284,839.00	G.V. Reklaitis Shell Companies Foundation, Inc. Shell Oil Company Foundation Fellowship	09/85-08/98
$60,000.00	G.V. Reklaitis E.I. DuPont de Nemours & Company E.I. DuPont de Nemours & Company Fellowship	09/81-09/97
$347,711.00	G.V. Reklaitis U.S. Department of Education Purdue Program for Graduate Assistance in Chemical Engineering Areas of National Need	09/97-08/99
$117,991.00	G.V. Reklaitis C.D. McAllister Endowment Goddard Fellowship	06/90-09/99
$314,725.00	G.V. Reklaitis National Consortium Graduate Minorities Engineering and Science National Consortium for Minorities Fellowship	09/92-09/98
$69,438.00	G.V. Reklaitis G.V Oak Ridge Associated Universities Computational Science Graduate Fellowship Program	09/92-08/97
$60,551.00	G.V. Reklaitis USDA Developing Environmentally and Economically Sustainable Food Processing Systems	09/95-09/98

Award Amount	PI/Sponsor/Title	Project Period
$213,600.00	E.M. Sevick-Muraca National Science Foundation National Young Investigator Biomedical Optical Imaging	09/94-09/98
$507,162.00	E.M. Sevick-Muraca Public Health Service N.H. Frequency-Domain Photon Migration Imaging for Breast Cancer Screening	08/94-05/98
$315,901.00	E.M. Sevick-Muraca Mallinckrodt Medical	08/94-09/98
$69,952.00	E.M. Sevick-Muraca University of Tennessee Process Monitoring with Measurement of Photon Migration	09/94-09/97
$285,245.00	E.M. Sevick-Muraca PHS-NIH National Cancer Institute Photon Migration Measurements for Tissue Diagnostics	07/95-07/99
$60,000.00	E.M. Sevick-Muraca E.I. duPont de Nemours & Co. Process Measurement	09/95-09/99
$337,328.00	E.M. Sevick-Muraca Public Health Service-NIH Frequency-Domain Lifetime Spectroscopy: A Tissue Phantom Study	09/96-08/98
$145,335.00	E.M. Sevick-Muraca Army Research Office Fluorescence Lifetime Imaging for Breast Cancer Detection and Diagnostics	07/96-06/98
$22,363.00	E.M. Sevick-Muraca Eli Lilly & Company Particle Size Research	03/97-09/99
$29,713.00	J.L. Sinclair National Science Foundation Presidential Young Investigator Award	09/97-02/99
$93,563.00	J.L. Sinclair Univ. Of Arizona - DOE Optimization of Coal Particle Flow Patterns in Low Nox Burners	10/97-01/00
$29,713.00	J.L. Sinclair Dow Chemical Company Research Support for Modeling Gas-Solid Flow area	12/97-09/99

Award Amount	PI/Sponsor/Title	Project Period
$10,000.00	J.L. Sinclair Chevron Research Co. Chevron - Grad Research	12/97-09/99
$11,666.00	V. Venkatasubramanian Purdue Research Foundation Automated Process Hazards Analysis of Batch Chemical Processing	09/97-09/98
$110,000.00	V. Venkatasubramanian Honeywell, Inc. A. Hybrid Intelligent System for Real-Time Process Fault Diagnosis	12/95-09/98
$195,351.00	V. Venkatasubramanian Lubrizol Corporation A Proposal to Develop a Neural Network-Genetic Algorithm Framework for Product Design and Formulation	12/95-12/98
$300,000.00	V. Venkatasubramanian National Science Foundation Process Systems Tools for the Development and Management of Environmentally and Economically Conscious Manufacturing	09/95-08/98
$80,000.00	V. Venkatasubramanian G.D. Searle & Company Preclinical Research & Development	05/96-09/99
$10,000.00	V. Venkatasubramanian Exxon Education Foundation Research in Real-Time Process Assessment	08/96-11/98
$50,000.00	V. Venkatasubramanian ICI Engineering Technology General Research in Process Safety Area	11/96-09/99
$17,000.00	N.-H.L. Wang Trask Trust Fund Beta-Site Testing and Further Development of Verse	01/93-07/97
$22,176.00	N.-H.L. Wang Purdue Research Foundation Design a New Adsorption Process for Removal of Organics from Water and Wastewater	01/96-01/98
$50,000.00	N.-H.L. Wang Showalter Trust Removal of Toxic Organics from Water and Wastewater	07/95-06/98
$162,436.00	N.-H.L. Wang Abbott Laboratories Model-based Design, Optimization, and Scale-up of Simulated Moving Bed	08/97-01/99

Award Amount	PI/Sponsor/Title	Project Period
	Chromatography for Antibiotics Recovery and Purification	
$43,163.00	N.-H.L. Wang GIST-Brocades Applications & Modifications of Verse for Process Design, Optimization and Scale up.	05/98-05/99
$11,666.00	N.-H.L. Wang Purdue Research Foundation Thermal Fractionation in Continuous Chromatography	05/98-05/99
$230,717.00	P.C. Wankat National Science Foundation Multicomponent Adsorption Processes	05/94-04/98
$21,928.00	P.C. Wankat Purdue Research Foundation Development of Simultaneous Fermentation/Separation from Lactic Acid Production	09/95-09/97
$55,556.00	P.C. Wankat National Science Foundation New Regeneration Methods for Adsorption	09/97-09/99
$11,666.00	P.C. Wankat Purdue Research Foundation Latent Heat Regeneration of Adsorbers	03/98-03/99

Thesis Projects

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Balasubramhanya, Lalitha *Doyle*	Low Order Models for Nonlinear Process Control	PhD August 8, 1997
Burgos-Rubio, Concepcion N. *Wankat/Okos*	Continuous Fermentation of Lactose for Lactic Acid Production by Simultaneous Bioreaction and Product Separation	PhD August 8, 1997
Doakes, Kelley P. *Andres*	Synthesis of a Metal / Ceramic Membrane for Oxygen Separation	MS August 8, 1997
Kendi, Thomas A. *Doyle*	Model-Based Control of Constrained Nonlinear Process Systems	PhD August 8, 1997
Kwatra, Harpreet *Doyle*	Neuro-Mimetic Dynamic Gain Scheduled Process Control	PhD August 8, 1997
Ostrowski, Mark H. *Lackritz*	Electric Field Effects in Polymer Thin Films for Second Order Nonlinear Optics	PhD August 8, 1997
Tsao, David Teh-Wei *Okos/Eckert*	Modeling the Environmentally or Biologically Controlled Nutrient Uptake Kinetics into Plants	PhD August 8, 1997
Wilkes, Edward D. *Basaran*	Finite Element Analysis of Forced Oscillations of Supported Drops	MS August 8, 1997
Byrne, Mark E. *Wankat*	Pressure Effects in Adiabatic Adsorption and Adsorptive Reactors	MS December 20, 1997
Chai, Lu *Basaran*	Fluid Mechanics of Distillation	MS December 20, 1997
Chen, Alvin Un-Teh *Sevick-Muraca*	Effects of Fluorescence and Phosphorescence Lifetime on Frequency Domain Optical Contrast for Biomedical Optical Imaging	MS December 20, 1997
Ernest, Jr., Michael V. *Wang*	Model-Based Design of Carousel Ion-Exchange Processes	PhD December 20, 1997
Liu, Jia *Andres*	Fabrication of 2-D and 3-D Nanocluster Networks	MS December 20, 1997
Lopez, Guadiana *Sevick-Muraca*	Absorption and Fluorescent Contrast Mechanisms for the Detection and Diagnosis of Breast Cancer Using Single-Pixel Frequency-Domain Photon Migration Imaging	MS December 20, 1997
Lowman, Anthony M. *Peppas*	The Dynamics of Complexation Graft Copolymers: Structural Analysis, NMR Spectroscopy and Their Implication for Biomedical Application	PhD December 20, 1997

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Matthews, Jonathan T. *Andres*	Design and Characterization of a Distributed Arc Cluster Source for Nanoparticle Synthesis	MS December 20, 1997
Pasmore, Jr., Tom A. *Lackritz*	The Effects of Polar Dopants in Polymers Subjected to Applied Electric Fields	PhD December 20, 1997
Randall, Daniel R. *Lackritz*	Monitoring and Analyzing Structural Relaxation Following Temperature Jumps in Doped Polymer Systems Using Second Harmonic Generation	MS December 20, 1997
Shin, Dongil *Venkatasubramanian*	Intelligent Tutoring System Framework for Operator Training in Process Fault Diagnosis	PhD December 20, 1997
Shrikhande, Prashant *Caruthers*	Prediction of Deformation and Enthalpy Relaxation for an Amorphous Polymer Using a Thermoviscoelastic Constitutive Model	MS December 20, 1997
Troy, Tamara L. *Sevick-Muraca*	Biomedical Optical Imaging From Frequency Domain Photon Migration Measurements: Experiments and Image Reconstruction	PhD December 20, 1997
Varner, Jeffrey D. *Ramkrishna*	Metabolic Engineering from a Cybernetic Perspective. A Conceptual Framework	PhD December 20, 1997
Wajge, Rajesh M. *Reklaitis*	Campaign Optimization of Multicomponent Reactive Batch Distillation	PhD December 20, 1997
Williams, Christopher T. *Takoudis*	Surface-Enhanced Raman Spectroscopy as an In-Situ Real-Time Probe of Heterogeneous Catalytic Reactions	PhD December 20, 1997
Wisnewski, Philip A. *Doyle*	Inferential Control Using High-Order Process Models with Application to a Continuous Pulp Digester	PhD December 20, 1997
Irwin, Nancy C. *Greenkorn*	Magnetic Resonance Imaging Experiments for the Verification of a Stochastic Transport Theory	PhD May 9, 1998
Keys, Kelley Britton *Peppas*	Poly(ethylene glycol) Star Polymer Hydrogels	MS May 9, 1998
Kim, Jum Sik *Basaran*	Effects of an Electric Field on the Deformation and Breakup of a Stretching Liquid Bridge	MS May 9, 1998
Kuo, Roger Keith Hiep *Greenkorn*	Experimental Verification of Nonlocal Dispersion Theory in Aperiodic Heterogeneous Porous Media	MS May 9, 1998

Graduate Student *Major Professor*	Thesis Title	Degree Date Granted
Manz, Thomas A. *Delgass*	Selective Hydrogenation of Butyronitrile on Promoted Raney® Nickel Catalysts	MS May 9, 1998
Novenario, Carlos Rull *Caruthers & Chao*	Phase Equilibria of Polymer Solutions Using the Chain-of-Rotators Equation of State	*PhD* May 9, 1998
Pirog, Theodore W. *Ramkrishna*	Dynamics of Destabilization of Food Emulsions. Measurement and Simulation of Gravity Driven Particle Velocities in Polydisperse Dispersions	PhD May 9, 1998
Scott, Robert A. *Peppas*	Highly Crosslinked Ionizable Acrylates: Polymerization Kinetics and Network Structure	PhD May 9, 1998
Srinivasan, Rajagopalan *Venkatasubramanain*	PHAzer: An Intelligent Multiple Models Based Process Hazards Analyzer	PhD May 9, 1998
Walters, William E. *Delgass*	The Effects of Cesiu m and Support on the Epoxidation of Ethylene	MS May 9, 1998
Xie, Yi *Wang*	Separation of Two Amino Acids Using SMB Chromatography	MS May 9, 1998

Course Offerings and Seminars 1997-1998