VIRGINIA TECH

Department of Chemical Engineering

Publications, Presentations, and Other Scholarly Activities

2003-2004
Academic Year
VT Chemical Engineering
Faculty Research Areas

Polymers & Polymer Processing
Wilkes, Baird, Davis, Marand, Kiran, Saraf, Liu

Advanced Materials Membranes
Marand, Oyama, Baird, Saraf

Biotechnology Tissue Engineering Biomedical Devices
Williams, Goldstein, Van Cott, Saraf

Catalysis & Surface Science
Oyama, Cox

Supercritical Fluids & High-Pressure
Kiran

Computational Science and Engineering
Cox, Liu

Nanotechnology Self-Assembly
Davis, Saraf, Marand

Computer-aided Design
Liu

Energy & Environment
Liu, Oyama, Baird

VT Chemical Engineering Department
Faculty

Donald G. Baird (Wisconsin)
Polymer processing, non-Newtonian fluid mechanics

David F. Cox (Florida)
Catalysis, ultrahigh vacuum surface science

Richey M. Davis (Princeton)
Colloids and polymer chemistry, nanostructured materials

Yasar Demirel* (U. Birmingham)
Applied thermodynamics, phase equilibria, design & simulations

Eva Marand (Massachusetts)
Transport through polymer membranes, polymer spectroscopy

S. Ted Oyama (Stanford)
Heterogeneous catalysis and new materials

Ravi F. Saraf (Massachusetts)
Nanotechnology, biomedical devices, polymers

Joseph T. Sullivan (Minnesota)
Marketing and chemical distribution

Kevin E. Van Cott (Virginia Tech)
Biotechnology, nanotechnology

Garth L. Wilkes** (Massachusetts)
Structure-property-processing behavior of polymeric materials

Yasar Demirel* (U. Birmingham)
Applied thermodynamics, phase equilibria, design & simulations

Evan S. Goldstein (Carnegie Mellon)
Tissue engineering, interfacial phenomena in bioengineering

Erdogan Kiran [Department Head] (Princeton)
Supercritical fluids, polymer science, high pressure techniques

Y.A. Liu (Princeton)
Pollution prevention and computer-aided design

* Visiting Professor
** University Distinguished Professor Emeritus

Research Centers and Focus Areas

Polymer Materials and Interface Laboratory
Center for Composite Materials and Structures
School of Biomedical Engineering and Science
Center for Self-Assembled Nanostructures and Devices
Biotechnology and Tissue Engineering
School of Biomedical Engineering and Science
Center for Self-Assembled Nanostructures and Devices
Biotechnology and Tissue Engineering
Surface Chemistry and Catalysis
Colloid and Surface Science
Computer-aided Design
Nanotechnology and Biomedical Devices
Supercritical Fluids and High Pressure Processing
Publications

Book Chapters:

**R.M. Davis**


**G.L. Wilkes**


Journal Publications

**D.G. Baird**


D.F. Cox


R.M. Davis

Y. Demirel


A.S. Goldstein

E. Kiran

Y.A. Liu


E. Marand


S.T. Oyama


**R.F. Saraf**


**K.E. VanCott**

**G.L. Wilkes**


K.F. Williams


Conference Proceedings

D.G. Baird


R.M. Davis

E. Kiran
S.T. Oyama


G.L. Wilkes


Presentations

Invited Presentations at Universities

D.G. Baird
“Assessing the Branching Structure of Polyethylene,” Tulane University, Department of ChE seminar, March 19, 2004.

E. Kiran
“Miscibility and Phase Separation in Polymer Solutions in Dense Fluids: Challenges and Opportunities,” Chemical Engineering Department, West Virginia University, Morgantown, West Virginia, March 5, 2004.

“High-pressure Miscibility and Phase Separation in Polymer Solutions,” Chemical Engineering Department, University of California at Los Angeles, May 7, 2004

Invited Presentations at Corporations

E. Marand

“Mixed Matrix and Nano-composite Membranes for Gas Separation Applications,” Sandia National Labs, Albuquerque, NM, 10/6/03.

Invited Presentations at Technical Meetings

D.G. Baird

The Use of Shear and Extensional Measurements in Identifying Branching, Conference sponsored by TA Instruments, San Antonio TX, February1-4, 2004.


E. Kiran
“High Pressure Miscibility and Phase Separation in Polymer Solutions. Challenges and Opportunities,” Invited Plenary lecture at the 5th Brazilian meeting on Supercritical Fluids, Florianopolis-SC- Brazil, April 22, 2004.

R.F. Saraf

Invited Cover Story

Y.A. Liu
Invited Workshop Participant

K.F. Williams


Presentations at Technical Conferences

D.G. Baird


D.F. Cox


Q. Ma, M.A. Minton and D.F. Cox, “Coupling and Decomposition of Surface Vinyl Species on Stoichiometric $\alpha$-Cr$_2$O$_3$ (10\_2),” 77th ACS Colloid and Surface Science Symposium, Atlanta, GA, June 2003.

C.M. Byrd, Q. Ma, M.A. Minton and D.F. Cox, “Reaction of Methyl Fragments on Stoichiometric $\alpha$-Cr$_2$O$_3$ (10\_2),” 77th ACS Colloid and Surface Science Symposium, Atlanta, GA, June 2003.
R.M. Davis


J. Krsmanovic, R.M. Davis, K.E. Van Cott, J.S. Riffle, “Adsorption of Water-Soluble Triblock Copolymers of Poly(ethylene oxide) and Carboxylic Acids on Silica And Alumina,” American Institute of Chemical Engineers Annual Fall 2004 meeting, November 17-29, 2003, San Francisco.


Y. Demirel
“Teaching Chemical Engineering Courses with Workbook Strategy,” ASEE, SE Section, Annual Conference, April 4-6, 2004, Auburn, AL.


“Nonequilibrium Thermodynamics and Stability Analysis of Transport and Rate Processes,” Third International Workshop on Nonequilibrium Thermodynamics and Complex Fluids, August 14-17, 2003, Princeton, NJ.

A.S. Goldstein


E. Kiran

E. Marand


S.T. Oyama


**R.F. Saraf**


**K.E. VanCott**


G.L. Wilkes


K.F. Williams


Outreach Activities – Workshops and Short Courses

R.M. Davis
“Waterborne Adhesives and Applications”, a section of the “Adhesion Science Short Course” for the Research Experience for Undergraduates (REU) program sponsored by the Center for Adhesive and Sealant Science (Virginia Tech) in cooperation with The Adhesive and Sealant Council Education Foundation, May 21, 2003. (25 attendees)

“Adhesive and Sealant Rheology” and “Waterborne Adhesives,” sections of the Adhesion Science Short Course, presented through the Center for Adhesive and Sealant Science (Virginia Tech) in cooperation with The Adhesive and Sealant Council Education Foundation, June 2-6, 2003. (34 attendees)


A.S. Goldstein


E. Kiran
Hosted Visiting Professor Sang-Do Yeo from Kyungpook National University, South Korea, who spent his sabbatical year at Virginia Tech.

Hosted two diploma students (Christopher Kornmeyer and Jan Koop) from Karlsruhe University in Germany.
Y.A. Liu

*International Outreach*

Formosa Petrochemical Corporation, Mailiao, Taiwan (March 8 to 12, 2004)
- Development of Butadiene Simulation Model,” and (b) “Water Savings in Refineries Using ASPEN WATER and WATER DESIGN.”

Formosa Petrochemical Corporation, Mailiao, Taiwan (January 5 to 16, 2004)
- Advanced Process Control Using Dynamic Matrix Control Plus (DMCplus)-Introductory Course; and (b) Advanced Process Control Using Dynamic Matrix Control Plus (DMCplus)-Advanced Concepts and Introduction to Inferential Property Development Using ASPEN IQ.

Beijing Yanshan Petrochemical Group and Aspen Tech Technical Service Center, Yanshan, Beijing, China (2003-2004)
- June 17 to 22, and July 22 to 27, 2003 (6 days at Yanshan; twice), (a) Process Simulation, Retrofit and Optimization Using ASPEN PLUS and (b) ASPEN PLUS Version 11 Updates for Version 10 Users.
- June 24 to 27, 2003 (4 days at Yanshan), Advanced Distillation with Applications to Chemical, Electrolyte and Petroleum Processes Using ASPEN PLUS.
- July 28 to July 5, 2003 (7 days at Yanshan), Simulation, Retrofit and Optimization of Large-Scale Ethylene Plants Using ASPEN PLUS.
- July 8 to 16, 2003 (8 days at Yanshan), Energy Savings in Process Industries Using ASPEN PINCH. ASPEN WATER and WATER DESIGN.
- July 17 to 20, 2003 (4 days at Yanshan), Water Savings in Ethylene, Refining and Chemical Plants Using ASPEN WATRER and WATER DESIGN.
- July 29 to August 3 (6 days at Yanshan), Simulation, Retrofit and Optimization of Large-Scale Polymer Plants Using PPOLYMERS PLUS.
- December 8 to 20, 2003 (12 days at Yanshan), (a) Advanced Process Control Using Dynamic Matrix Control Plus (DMCplus)-Introductory Course; and (b) Advanced Process Control Using Dynamic Matrix Control Plus (DMCplus)-Advanced Concepts and Introduction to Inferential Property Development Using ASPEN IQ.

SINOPEC Corporation (China) and Formosa Petrochemical Corporation (Taiwan)
- Led three visiting engineering teams from SINOPEC Corporation and Formosa Petrochemical Corporation to develop here at Virginia Tech (1) the steady-state and dynamic simulation models for a commercial, solid-state PET polymerization process; (2) water saving in refineries at Mailiao, Taiwan, with a capacity totaling 21 million tons of crude oil refined per year; and (3) the model-predictive control of ethylene plants using DMCplus, Aspen IQ and Aspen IQ Powertools.
Local Industries Outreach: Alliant Techsystems, Radford, Virginia

- Led 14 chemical engineering seniors of 2003-2004 to successfully complete five six sigma projects for process improvement and development with significant economic payback and environmental benefits.
- “Economical and Green Process for Producing Diethylene Glycol Dinitrate.”
- “Cooling Condenser Redesign” (Recommendation already implemented)
- “Improve the Homogeneity of Solid Mixing Using Double-Cone Blenders” (Recommendation already implemented)
- “Selective Catalytic Reduction (SCR) Unit Ammonia Injection Modeling and Control Strategy Development” (Control system already implemented)
- “Efficiency Optimization of the Acidic Wastewater Lime Neutralization Process” (Recommendation already implemented)

Outreach to Virginia Industries-Honeywell Specialty Materials

- Technology development and engineering training in computer-aided process modeling for Honeywell Nylon, Inc.

G.L. Wilkes

- Principles and Practices of Polymer Chemistry, taught 2-3 times per year in Blacksburg – ca. 30 participants per course. (5 day course) (Wilkes, McGrath, Long, Ward, Riffle)
- Introduction to Polymeric Adhesives and Composites, taught once per year in Blacksburg – ca 25 participants per course. (5 day course) (several lecturers)
- Dupont Polymer Short Course, August 2003.

K.F. Williams

Teacher Link Fellow – Teacher Link Program (TLP), North Carolina Science, Mathematics, and Technology Education Center (June 2003-June 2004)

Software/Patents

E. Marand

VTIP no 01.047 Disclosure “A Method of the Fabrication of a Novel Polymer/Porous Layered Materials Nanocomposite Films and their Applications.”

S.T. Oyama

R.F. Saraf


Journal Editorships

E. Kiran
*Journal of Supercritical Fluids*

G.L. Wilkes
Co-editor, *Journal of Macromolecular Science*

Journal Editorial Board Memberships

D.G. Baird
*Advances in Polymer Technology*

E. Kiran
Turkish *Journal of Engineering and Environmental Sciences*

S.T. Oyama
*Journal of Natural Gas Chemistry*

G.L. Wilkes
*Journal of Applied Polymer Science*  
*Reviews on Polymer Research and Engineering*  
*Journal of Polymer Engineering*  
*Journal of Inorganic and Organo-Metallic Polymers*

K.F. Williams
*Journal of Theoretical Biology*

Conference Organization

A.S. Goldstein

Honors and Awards

D.G. Baird
International Award for Research, Society of Plastics Engineers, 2003.

S.T. Oyama
Virginia Tech, College of Engineering, Dean’s Award for Research, 2004.

G.L. Wilkes
Co-recipient of the Flory Award in Polymer Education [with J. McGrath and T. Ward in the Department of Chemistry at Virginia Tech], presented at the 2004 Spring American Chemical Society Meeting.

Departmental Seminars

Fall 2003

September 15
Kumar Malikarjunan, Biological Systems Engineering, Virginia Tech
“Challenges for a Better Food Supply in Coming Years – Role of Chemical Engineers”

September 22
Mike Bortner, PhD Student, Chemical Engineering Department, Virginia Tech
“Melt Processable Acrylic Copolymers”

October 3
Jefferson Tester, Chemical Engineering Department, MIT
“The Role of Multiscale Chemical Thermodynamics in Modeling Gas Hydrate Systems”

October 17
Patricia M. Dove, Department of Geological Sciences, Virginia Tech
“Investigating the Physical Basis of Biomineralization”

October 24
Christopher Jones, School of Chemical Engineering, Georgia Institute of Technology

October 31
Ilhan Aksay, Chemical Engineering Department, Princeton University
“Self-Healing Organic/Inorganic Composites”

November 7
Peter Cummings, Chemical Engineering Department, Vanderbilt University
“Computational Nanoscience”
November 10
**Hassan Aref**, Dean, College of Engineering, Virginia Tech
“Modeling the Structure and Dynamics of a Dry Foam”

December 1
**Sanjun Niu**, PhD Student, Chemical Engineering Department, Virginia Tech
“A Label-Free Method to Decipher DNA Sequence”

December 8
**Jay Khare**, PhD Student, Chemical Engineering Department, Virginia Tech
“A Reactor Model for Metallocene-Catalyzed Ethylene Polymerizations”

**Spring 2004**

February 16
**John Walz**, Chemical Engineering, Yale University
“Control of Colloidal Stability Using Nonadsorbing Polyelectrolytes”

February 24
**Johanna M.H. Levelt Sengers**, National Institute of Standards and Tech.
“Key Concepts from Gibbs that Empowered Van der Waals, Korteweg and Kamerlingh Onnes”

March 16
**Amadeu Sum**, Chemical Engineering Department, University of Wisconsin
“Stability and Structure of Phospholipid Bilayer Systems: A Molecular Perspective on the Mechanisms of Preservation”

March 26
**Jingguang Chen**, Center for Catalytic Science & Technology, Univ. of Delaware
“Understanding and Predicting Catalytic Properties of Bimetallic Catalysts from Experiments and DFT Modeling”

April 9
**Nicholas Abbott**, Dept. of Chemical Engineering, University of Wisconsin
“Biomolecular Interactions at Phospholipid-Decorated Surfaces of Thermotropic Liquid Crystals”

April 20
**Eric Scribben**, PhD Student, Chemical Engineering Department, Virginia Tech
“Rotational Molding of Thermotropic Liquid Crystalline Polymers”

April 23
**John Rabolt**, Materials Science and Engineering, University of Delaware
“Characterization of Changes in Conformational Order in Polymer Nanofibers and Langmuir Blodgett Films Caused by Direct and Self-Assembly”
April 27
**William Schneider**, Ford Motor Company
“Insights from First Principles into the Unusual Catalytic Reactivity of NOx”

May 4
**Todd Pechar**, PhD Student, Chemical Engineering Department, Virginia Tech
“Fabrication and Characterization of Polyimide-based Mixed Matrix Membranes for Gas Separations”

**Active Projects During the Academic Year 2003-2004**

**D. G. Baird**

- **Sponsor:** Luna Innovations, Inc
  **Project Title:** Rotational Molding of Thermoplastic Cryogenic Propellant Tasks

- **Sponsor:** EPA
  **Project Title:** Benign Processing of Polymers Plasticized with Absorbed Carbon Dioxide

- **Sponsor:** Daimler Chrysler Corp
  **Project Title:** Injection Molding of Wholly Thermoplastic Composites

- **Sponsor:** DOE
  **Project Title:** Advanced Materials for PEM-Based Fuel Cell Material Systems

- **Sponsor:** VPI Foundation
  **Project Title:** Industrial Account/Kodak, Extension Rheology

**D. F. Cox**

- **Sponsor:** Department of Energy
  **Project Title:** Influence of Surface Defects and Local Structure on Chemisorption Properties and Oxidation Reactions over Metal Oxide Surfaces

**R. M. Davis**

- **Sponsor:** Luna Innovations, Inc
  **Project Title:** Novel Water Soluble TNT Metallofullerene Derivatives for Imaging Applications – Phase I

- **Sponsor:** NSF
  **Project Title:** Monodisperse Block Copolymers for Environmentally-friendly Processing of Aqueous Metal Oxide Suspensions
Sponsor: VPI Foundation  
Project Title: Colloid Stabilization Research

Sponsor: Luna  
Project Title: Fluorescent, Polymerized, Affinity Liposomes for the Detection of Bacterial Toxins

Sponsor: Luna  
Project Title: Viability Assays for Monitoring Decontamination of Pathogenic Bacteria

**A. S. Goldstein**

Sponsor: OSER  
Project Title: Hemocompatible Tubing Coatings Fabricated by the Electro-Static Self-Assembly Process

Sponsor: NIH  
Project Title: Characterization of Shearing Flow as an Osteoinductive Stimulus for Bone Tissue Engineering

Sponsor: Rockefeller Brothers Fund  
Project Title: Micron-Scale Substrate Topographies for Contact Guidance (?) and Bone Tissue Engineering

**E. Kiran**

Sponsor: VPI Foundation  
Project Title: Polymer Processing in or with Supercritical Fluids

**Y. A. Liu**

Sponsor: VPI Foundation  
Project Title: Polymer Process Modeling

Sponsor: VPI Foundation  
Project Title: Computer Aided Design

**E. Marand**

Sponsor: NSF  
Project Title: The Development of Mixed Matrix Membranes

Sponsor: NSF  
Project Title: Polymide-Silica Hybrid
Sponsor: Sandia National Lab.
Project Title: Ladder Polymer Structure-Property Study

Sponsor: VPI Foundation
Project Title: Dupont Research

S. T. Oyama

Sponsor: NSF
Project Title: Catalytic Membrane Technology for the Conversion of Greenhouse Gasses

Sponsor: Department of Energy
Project Title: Bimetallic Oxycarbides and Oxynitrides a new class of Hydrogenation Catalysts

Sponsor: Conoco
Project Title: Catalytic Membrane Technology for the Conversion of CH4 and CO2

Sponsor: New Energy Development
Project Title: Catalysts for Ultra-Clean Fuels

Sponsor: VPI Foundation
Project Title: Carbine & Nitrides Research

Sponsor: NSF
Project Title: Kinetics and Mechanism of Catalytic Oxidation with Ozone

Sponsor: NSF
Project Title: Kinetics and Mechanism of Catalytic Oxidation with Ozone-Ren Supplement

R. F. Saraf

Sponsor: Office of Naval Research
Project Title: Piezo Electric/Piezo Optical Large Area Thin Film Device of Pressure Imaging and Sensing

Sponsor: OSER
Project Title: Sequencing Untagged DNA and Proteins-A Multimodal Microarray Chip

Sponsor: VPI Foundation
Project Title: Physical and Biological Science
Sponsor: NSF  
Project Title: Nanodevice for Imaging Normal Stress Distribution with Application in Sensing Texture and “fee” by Touching

**G. L. Wilkes**

Sponsor: US Army Research Office  
Project Title: Fundamental Investigations of Tailored Macromolecular Topology and Chemical Reactivity

Sponsor: Urethane Soy Systems  
Project Title: Polyurethanes for Soy Bean Oil: Synthesis, Chemical Analysis and Structure Property Behavior

Sponsor: VPI Foundation  
Project Title: Polymer Materials and Interfaces Laboratory

Sponsor: VPI Foundation  
Project Title: Millennium Account

Sponsor: VT Educ FDN  
Project Title: Chemical Engineering Industrial Research

**K. F. Williams**

Sponsor: Boston University School of Medicine  
Project Title: Control of Vascular Smooth Muscle Cell Proliferation

Sponsor: University of Arkansas  
Project Title: Mechanisms of Golgi: Apparatus Protein Recycling-Computational Supplement

Sponsor: NSF  
Project Title: Career: Growth Factor Accessibility and the Role of Extracellular Mediators

Sponsor: NIH  
Project Title: Chondrocytes: Mechanical Hormonal Mediated Response

Project Title: Industrial Support

Sponsor: Carilion Biomedical Institute  
Project Title: Production of Recombinant Procine Relaxin Variants and Evaluation in Angiogenesis and Wound Healing Models
Sponsor: Commonwealth Health Research Board
Project Title: Ph-dependent Regulation of IGF-1 Stimulation by IGFB P-3

Graduate Degrees Granted

December 2003 Commencement

Michael Bortner
PhD Advisor: Don Baird
Dissertation title: Melt Processing of Thermally Unstable Acrylic Copolymer Precursors

Chad Byrd
PhD Advisor: David Cox
Dissertation title: The Reaction of C1 Hydrocarbons on Cr2O3 (10̈1 2)

Matthew Guzy
PhD Co-Advisors: Richey Davis, Kevin Van Cott

Doug Henderson
Co-Advisors: Kevin Van Cott, Rick Davis
Report title: Development of Novel Cloning Strategies for the Production of Surface-Active Poly (amino acids)

Michael Hickner
PhD Co-Advisors: Garth Wilkes, James McGrath (Chem)
Dissertation title: Structure and Transport in Fuel Cell Proton Exchange Membranes

Neeraj (Jay) Khare
MEng Advisor: Y. A. Liu
Report title: Predictive Modeling of Metal-Catalyzed Polyolefin Processes
PhD Advisor: Y. A. Liu
Dissertation title: Predictive Modeling of Metal-Catalyzed Polyolefin Processes

Wojtek Krych
MS Advisor: Eva Marand

Yong Kul Lee
MEng Advisor: S. Ted Oyama
Report title: A Novel Zeolite-Supported Phosphide Catalyst for Deep Hydrodesulfurization

Myles Lindsay
MEng Advisor: Kevin Van Cott
Report title: Purification and Characterization of Recombinant Human Factor IX Produced in the Milk of Transgenic Pigs
Emmett O’Brien  PhD Advisor: Tom Ward (Chem)
Dissertation title: Durability of Adhesive Joints Subjected to Environmental Stress

Julie Davis Paye  PhD Advisor: Kim Williams
Dissertation title: Effects of the Insulin-Like Growth Factor (IGF) Axis on the Transport Properties of Endothelial and Epithelial Cells In Vitro

Niloofar Rahmani  MEng Advisor: Eva Marand
Report title: Mixed Matrix Membranes: A Review

May 2004 Commencement

Michelle Kreke  MEng Advisor: Aaron Goldstein
Report title: Application of Fluid Flow for Functional Tissue Engineering of Bone Marrow Stromal Cells

Corey Reed  MEng Advisor: Ted Oyama
Report title: VOC Catalytic Oxidation on Manganese Oxide Catalysts Using Ozone
Chemical Engineering

Class of 2004
Chemical Engineering transforms our basic knowledge in chemical, physical, biological and life sciences to products and processes that benefit society.