James R. Fair Process Science and Technology Center

Winter 2016 Newsletter

http://dept.ceer.utexas.edu/ceer/pstc/

TEXAS
The University of Texas at Austin

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Note from the Program Head

Greetings from Austin. In an effort to enhance our contact with PSTC / SRP sponsors and friends, we are initiating a quarterly newsletter. Our goal would be to give our sponsors a view into the program which will supplement meetings and web postings. The program works best with a high degree of engagement between the research groups and our industrial friends and given the constraints on travel we thought it appropriate to assist in strengthening that connection. The newsletter consists of several sections highlighting PIs, graduate students, ongoing projects, and publications. I am certainly open to your suggestions for additional content.

The program continues to maintain a positive connection with industry and government funding sources. As I noted during the fall sponsors' meeting, there are multiple initiatives from DOE and NSF which cover research areas we have been at the forefront of investigating during the PSTC / SRP's thirty-two years of operation. It is rewarding to see that, despite the appropriate focus on new emerging technologies, the federal government still values traditional process engineering research. Our sponsorship headcount remains stable at around fifteen companies and the SRP contract research program works with another ten to fifteen each year. This contact maintains our focus on industrially relevant applied research while also informing the fundamental investigation of process technologies.

Our research focus continues to expand into new areas while maintaining support for critical existing technologies. We continue to be interested in the intersection of chemical reactions and separations technology. Our ongoing research program in CO_2 capture is an example of the expertise we can bring to such an effort. We would be interested in discussing other applications of the combined approach with our sponsorship. I published a review paper on olefin / paraffin separation in 1992 – unfortunately it is still cited as a source of technology options and the chemical industry is still refrigerating massive amounts of light gases in order to recover ethylene and propylene. One would think there has to be a better approach involving an olefin complexing agent. Water purification will be critical as we move into the twenty-first century. Applications ranging from agriculture to hydrocarbon reservoir injection will strain an already scarce commodity. Our ongoing efforts to utilize novel membrane approaches to address

this challenge are at the forefront of water purification research. Advanced process control is a low-cost option for enhancing process performance and our ongoing partnership with Emerson Process Management greatly enhances our ability to make a major impact in this area. The size of the SRP pilot plant allows us to conduct experiments near industrial scale and the advanced control system facilitates smooth operation and data collection while allowing novel control methodologies to be tested. Our current dividing wall distillation column study conducted utilizing Emerson's wireless data acquisition and control hardware and software is an excellent example of this capability.

While we are very proud of our researchers, we continue to look for emerging areas that will build on and extend our existing expertise. Our recent initiative with the University of California group at the leading edge of Metal Organic Framework (MOF) research is an example. We believe there is a high potential for synergy between the very scientific understanding Berkeley has developed and our ability to address application-related questions. I would welcome input from our sponsors on areas of high opportunity for this novel material.

We look forward to seeing you at the PSTC spring meeting (March 30th and 31st). As I mentioned above, our researchers, and more importantly our students, benefit from interaction with our very knowledgeable sponsor representatives. We have placed the meeting at the end of the San Antonio Spring AIChE meeting March 26th – 30th) with the hope of providing one-stop shopping for separations technology. The Henry Kister Distillation symposium will be held at the San Antonio meeting and I would encourage you to travel north on I-35 to visit Austin at the end of the week.

Best wishes,

Bruce

PI Spotlight: Frank Seibert

Having fun at one's job is frequently a rare gift, one that Frank Seibert is blessed to have. With more than three decades at the University of Texas at Austin (UT Austin) under his belt, Frank has combined his interests with plenty of enthusiasm for productive and fulfilling work in separations research.

A sixth generation Texan, Frank traces his roots back to 1820s Matagorda County where his ancestors originally settled. Frank himself came of age in the nearby Houston environs, eventually attending the University of Houston, graduating in 1982 with a B.S. in Chemical Engineering. Although he had originally wanted to be a marine biologist, his enjoyment of applied math and science and the jobs then available in Houston encouraged him to pursue chemical engineering instead.

With valuable undergraduate experience in liquid-liquid extraction, Frank was drawn to the Chemical Engineering Department at UT Austin by Professor James Fair to work with the department's brand-new, skid-mounted, controlled cyclic liquid extraction system and first computer-controlled equipment. The first major project Frank worked on was studying the performance of a controlled cyclic liquid-liquid extractor. This lead to his Ph.D.-earning study of structured packings in liquid-liquid extraction. Frank picked up an M.S. degree in 1984 followed by a Ph.D. in 1986.

By this time, the Separations Research Program had relocated from UT's main campus out to the Balcones (now Pickle) Research Campus. Frank, along with fellow graduate student Bruce Eldridge, was among the first four students in the new building. Construction of the new pilot plants was nearly complete, two of which were to involve extraction. The first computer-controlled supercritical extraction with solvent recovery by distillation was available—since supercritical extraction was a hot area of research in the 1980s, this equipment attracted visitors from around the world. Fair and Jose Bravo asked Frank to stay an extra year to get the systems up and running. Frank

agreed to the challenge, launching a 30-year career here at the Separations Research Program (SRP) and Process Science and Technology Center (PSTC). He enjoyed working with Bravo and Fair along with Dr. Jimmy Humphrey in new separations areas. Frank credits these three men with having the most impact on his career and with teaching him that chemical engineering could be fun.

Frank is currently working on four areas of research: enhancing understanding of sieve tray extractor hydraulics and mass transfer; developing improved mass transfer and pressure drop models for packed distillation and absorber columns; developing a membrane-based method to coalesce and remove micron-sized oil drops from water in the presence of solids; and, in collaboration with Eldridge and Dr. Michael Baldea, developing an improved understanding and control of Dividing Wall Distillation columns. Frank is also interested in applying the group's membrane-based process to bio-processes and fermenters.

The field of separations research has come a long way over the years, but liquid extraction remains a vital bulk separation method in chemical and petrochemical industries. Today's companies are always looking to increase throughput with minimal expense, and from time to time the liquid extractor is the bottleneck preventing progress. Coalescers and high-performance trays and packings are under evaluation for increasing capacity. Liquid extraction is also on the rise in companies that manufacture chemicals from biological feedstocks.

When considering the future of separations and the process science field, Frank states that chemical separation experience will always be in demand. Even two to three decades from now, bulk chemical separations will still be accomplished using distillation and extraction/distillation processes. He is hopeful that more governmental research funds will be directed towards separations; having that funding available to train graduates to take over for retiring experts is critical.

Of course, one cannot live on chemical engineering alone. Frank finds balance and relaxation wade-fishing the middle Texas coastal bays. He tackles the extraction of redfish and speckled trout with the same enthusiasm and joy that he brings to separation research. SRP and PSTC are very fortunate indeed to have Frank as a long-term and integral member of the team.

—Lauren Murrah

Student Spotlight: Jovan Kamcev

Our student spotlight this season falls upon Jovan Kamcev, recent graduate with a Ph.D. in Chemical Engineering and a longtime member of Dr. Benny Freeman's membrane research group. Originally hailing from Macedonia, a small country in Eastern Europe, he came to America in 2001 at age 12, joining his single mother who had immigrated four years prior to search for a better life for her and her son. Jovan immersed himself in American life and learned English by watching television and attending middle and high school in New York City. While studying at the highly ranked Brooklyn Technical High School, he experienced his first taste of scientific research while his mother worked as a researcher in biochemistry at Columbia University Medical Center. Jovan worked in an organic chemistry lab there during his summers and, as a result, his interest in science, particularly chemistry, grew.

After completing a chemistry major at his technical high school, Jovan entered Stony Brook University on Long Island and continued his studies in chemistry and math. His friends suggested combining his interest in chemistry and math and trying chemical engineering. The combination was a hit and he pursued a double major in chemical engineering and applied

mathematics and statistics. He added valuable research experience by working with a biomedical engineering research group at the university, going on to coauthor two papers with the group.

Jovan's interest in the materials field sparked during his summer job at Brookhaven National Laboratory (BNL) where he worked with inorganic materials and polymers. He published his first work as primary author during his senior year while at BNL. At this point in his studies and work, it was crystal clear to Jovan that he wanted to continue fundamental scientific research and the next step would be to pursue a doctoral degree.

Jovan applied to several graduate schools with the University of Texas at Austin's chemical engineering department emerging as the clear winner. The prominence of the department and the outstanding group of professors and researchers in the polymer area, in addition to Austin's great weather and natural surroundings, made UT Austin irresistible. He won a National Science Foundation graduate research fellowship to support financially his studies. Jovan joined Dr. Freeman's group with a focus on studying water and ion transport in ion exchange membranes for desalination and energy purification applications.

Although Jovan's original plan was to graduate in May 2017, he finished well ahead of his timetable, recently earning his Ph.D. in Chemical Engineering. He is currently a postdoctoral fellow in Dr. Freeman's group and has plans to pursue another postdoctoral position at different institution next summer before going on to an academic career. This has been an extraordinary journey for Jovan, from the small country of Macedonia to the enormous city of New York, from the hill country of Texas to a bright future in academia. We wish Jovan much success in his future as a chemical engineer.

—Susan Tedter and Lauren Murrah

Jovan Kamcev with his advisor Benny Freeman and his mother Stanka Semova .

Articles We've Published (2016)

Full citations and abstracts are available on the PSTC website.

Eldridge Group

- Dividing wall column control: common practices and key findings.

El-Halwagi Group

- A return on investment metric for incorporating sustainability in process integration and improvement projects.
- A shortcut approach to the multi-scale atomic targeting and design of c-h-o symbiosis networks.
- A shortcut approach to the design of once-through multi-stage flash desalination systems.
- Qatar's chemical industry: monetizing natural gas to the world.
- Optimization of the production of syngas from shale gas with economic and safety considerations.
- A review of biodiesel production from microalgae.
- Optimal design of multi-plant cogeneration systems with uncertain flaring and venting.
- Multi-objective optimization of dual-purpose power plants and water distribution networks.
- Optimal reuse of flowback wastewater in hydraulic fracturing including seasonal and environmental constraints.

- Optimization of synthetic jet fuels aromatic/paraffinic composition via experimental & property integration methods.
- A review of safety indices for process design.
- Optimal design of integrated solar power plants accounting for the thermal storage system and CO_2 mitigation through an algae system.
- Involving economic, environmental, and safety issues in the optimal purification of biobutanol.
- Simultaneous synthesis of utility system and heat exchanger network incorporating steam condensate and boiler feedwater.
- Mathematical optimization of a supply chain for the production of fuel pellets from residual biomass.
- Optimal planning and infrastructure development of shale gas.
- Fuzzy mixed integer non-linear programming model for the design of an algae-based eco-industrial park with prospective selection of support tenants under product price variability.
- Using module-based learning methods to introduce sustainable manufacturing in engineering curriculum.
- Integration of energy and wastewater treatment alternatives with process facilities to manage industrial flares during normal and abnormal operations—a multi-objective extendible optimization framework.
- Safety and techno-economic analysis of ethylene technologies.
- Optimal water management under uncertainty for shale gas production.
- Optimal synthesis of refinery property-based water networks with electrocoagulation treatment systems.
- Optimal reconfiguration of a sugar cane industry to yield an integrated biorefinery.
- Optimization across water-energy nexus for integrating heat, power, and water for industrial processes coupled with hybrid thermal-membrane desalination.
- On the identification of optimal utility corridor locations in interplant water network synthesis.
- Synthesis of industrial park water reuse networks considering treatment systems and merged connectivity options.
- Optimal location of biorefineries considering sustainable integration with the environment.
- A fuzzy mixed-integer linear programming model for optimal design of polygeneration systems with cyclic loads.

Freeman Group

- Analysis of the transport properties of thermally rearranged (TR) polymers and polymers of intrinsic microporosity (PIM) relative to upper bound performance.
- Influence of polydopamine deposition conditions on hydraulic permeability, sieving coefficients, pore size and pore size distribution for a polysulfone ultrafiltration membrane.
- The effect of permeate flux on membrane fouling during microfiltration of oily water.
- Surface modification of water purification membranes: a review.
- Non-equilibrium lattice fluid modeling of gas solubility in HAB-6FDA polyimide and its thermally rearranged analogs
- Gas transport properties and characterization of UV crosslinked poly(phenylene oxide-co-arylene ether ketone) copolymers.
- Liquid methanol sorption, diffusion and permeation in charged and uncharged polymers.
- Gas permeation and selectivity of poly(dimethylsiloxane)/graphene oxide composite elastomer membranes.
- Gas permeation properties of thermally rearranged (TR) isomers and their aromatic polyimide precursors.
- Fouling propensity of a poly(vinylidene fluoride) microfiltration membrane to several model oil/water emulsions.
- Charged polymer membranes for environmental/energy applications.
- Effect of polydopamine deposition conditions on polysulfone ultrafiltration membrane properties and threshold flux during oil/water emulsion filtration.
- Cracks help membranes to stay hydrated.
- Influence of toluene on CO_2 and CH_4 gas transport properties in thermally rearranged (TR) polymers based on 3,3'-dihydroxy-4,4'-diamino-biphenyl (HAB) and 2,2'-bis-(3,4-dicarboxyphenyl) hexafluoropropane dianhydride (6FDA).

- Synthesis and gas permeability of highly elastic poly(dimethylsiloxane)/graphene oxide composite elastomers using telechelic polymers.
- Effect of UV irradiation and physical aging on O_2 and N_2 transport properties of thin glassy poly(arylene ether ketone) copolymer films based on tetramethyl bisphenol a and 4,4'-difluorobenzophenone.
- Partitioning of mobile ions between ion exchange polymers and aqueous salt solutions: importance of counter-ion condensation.
- Underwater superoleophobic surfaces prepared from polymer zwitterion/dopamine composite coatings.
- Cross-linked disulfonated poly(arylene ether sulfone) telechelic oligomers. 2. elevated transport performance with increasing hydrophilicity.
- Highly CO_2-selective gas separation membranes based on segmented copolymers of poly(ethylene oxide) reinforced with pentiptycene-containing polyimide hard segments.
- Gas permeation and mechanical properties of thermally rearranged (TR) copolyimides.

Long Group

- Enhanced ethylene separation and plasticization resistance in polymer membranes incorporating metal-organic framework nanocrystals.
- Plasticization-resistant Ni_2(dobdc)/polyimide composite membranes for the removal of CO_2 from natural gas.
- Reversible CO scavenging via adsorbate-dependent spin state transitions in an iron(II)-triazolate metal-organic framework.
- Selective, tunable O_2 Binding in cobalt(II)-triazolate/pyrazolate metal-organic frameworks.
- Olsalazine-based metal-organic frameworks as biocompatible platforms for H_2 adsorption and drug delivery.
- Pore environment effects on catalytic cyclohexane oxidation in expanded Fe_2(dobdc) analogues.
- Tuning the methane adsorption-induced phase change in the flexible metal-organic framework Co(bdp).
- Hydrogen storage and selective, reversible O_2 adsorption in a metal-organic framework with open chromium(II) sites.
- Hydrogen storage in the expanded pore metal-organic frameworks M_2(dobpdc) (M = Mg, Mn, Fe, Co, Ni, Zn).
- Adsorption of two gas molecules at a single metal site in a metal-organic framework.

Ritter Group

- Ideal cascade theory applied to carbon monoxide isotope separation by pressure swing adsorption.

Rochelle Group

- Approaching a reversible stripping process for CO_2 capture.
- A review of conventional amine scrubbing for CO_2 capture.
- Thermodynamics of aqueous methyldiethanolamine/ piperazine for CO_2 capture.
- Kinetics of aqueous methyldiethanolamine/piperazine for CO_2 capture.
- Thermal degradation of novel piperazine-based amine blends for CO_2 capture.
- Control relevant model of amine scrubbing for CO_2 capture from power plants.
- Dynamic modeling and control of an intercooled absorber for post-combustion CO_2 capture article.
- Dimensionless models for predicting the effective area, liquid-film, and gas-film mass-transfer coefficients of packing.
- Regulatory control of amine scrubbing for CO_2 capture from power plants.
- Effectiveness of absorber intercooling for CO_2 absorption from natural gas fired flue gases using monoethanolamine solvent.

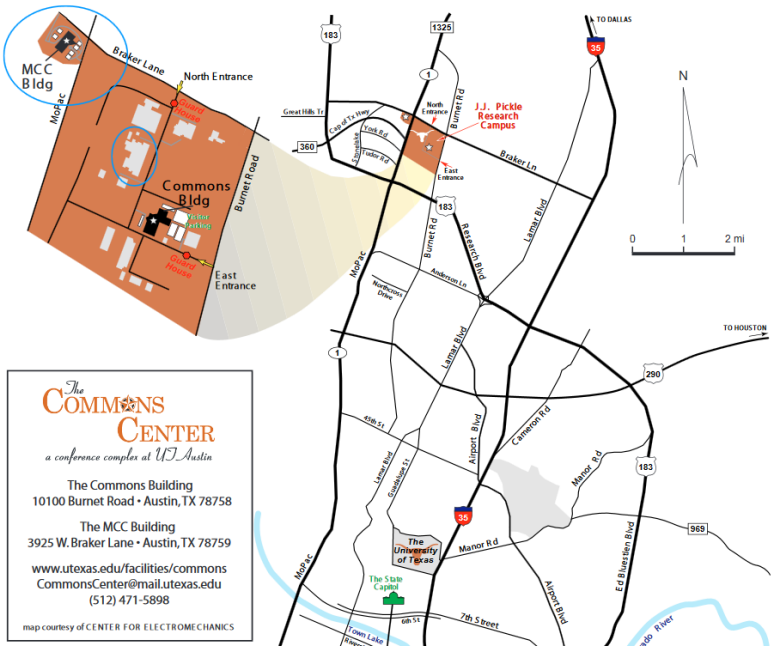
- Thermodynamic and mass transfer modeling of carbon dioxide absorption into aqueous 2-piperidineethanol.
- Thermodynamic and mass transfer modeling of carbon dioxide absorption into aqueous 2-amino-2-methyl-1-propanol.
- Comment on "Reassessing the efficiency penalty from carbon capture in coal-fired power plants."
- Thermal degradation of piperazine/4-hydroxy-1-methylpiperidine for CO_2 capture.
- Capacity and absorption rate of tertiary and hindered amines blended with piperazine for CO_2 capture.
- Absorber modeling for NGCC carbon capture with aqueous piperazine.
- Pilot plant test of the advanced flash stripper for CO_2 capture.
- Process control of the advanced flash stripper for CO_2 solvent regeneration.

Seibert Group

- Dimensionless models for predicting the effective area, liquid-film and gas-film measurements.
- Effect of liquid viscosity on liquid phase mass transfer coefficient for GT-OPTIMAK 250Y.
- Liquid-liquid extraction and other liquid-liquid operations and equipment.

Spring 2017 Meeting

Please join us for our annual PSTC Spring Meeting March 30-31, 2017, here at the University of Texas at Austin. Once again, we will be at the Commons Learning Center located on the Pickle Research Campus. Registration and accommodation information are available on our website. Handouts of the presentations will be available for attendees; pdf copies will be posted on our website closer to meeting time.



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