James R. Fair Process Science & Technology Center

TEXAS The University of Texas at Austin

Fall 2021 Newsletter

In This Issue:

Note from the Program Head

https://sites.utexas.edu/pstc/

Alas, I am still writing PSTC program head notes from the home office. There is some good news—we are returning to a slightly more normal mode of course instruction. I have divided my senior design class into three cohorts who attend live, in the classroom, instruction once a week. The non-classroom participants still watch the lectures on ZOOM. It would have been easier to mask and vaccinate everybody, but I won't politicize this note.

The PSTC / SRP appears to have weathered the storm. We only lost one PSTC sponsor and Frank's operation made it through the worst downturn in the program's history with financial help from several of our industrial sponsors and the UT Engineering School. This support was much appreciated. The end of 2021 and 2022 appears to be returning to the "normal" level of research activity.

I am excited about the opportunity to address the challenges the refining and chemical industry will face over the next decade. Plastic recycling, CO2 emission reduction, and carbon capture and storage are major challenges that the PSTC / SRP researchers can help address. These critical areas will also require well trained engineers, a commodity we supply as well as any institution. My assessment is that federal funding sources will be under increasing pressure so industrial support will become increasingly important for the research we conduct.

The fall PSTC meeting will be held on Tuesday, October 19th and Wednesday, October 20th. We had hoped to have an in-person meeting but the pandemic conditions will, in all probability, prevent that approach. Our virtual meeting platform is ZOOM which appears to not be causing any unworkable issues with corporate firewalls. A major benefit of ZOOM is cloud recording which has been a great way for our sponsors to distribute meeting information throughout their organizations.

As always, thanks for the support. Please contact me with any questions.

Best wishes and stay safe,

Bruce

SRP Update: Frank Seibert

After numerous modifications, the SRP pilot plant is preparing for a three-month pilot plant carbon dioxide campaign which will focus on developing an improved understanding of solvent oxidation. The project is part of Professor Gary Rochelle's US Department of Energy Contract. The pilot plant study will complement several PhD lab-scale studies also focusing on reducing solvent oxidation.

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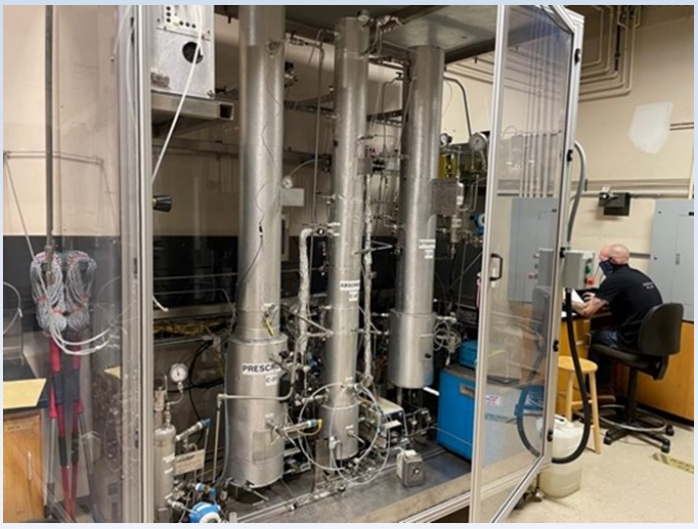
SRP Update Cont.

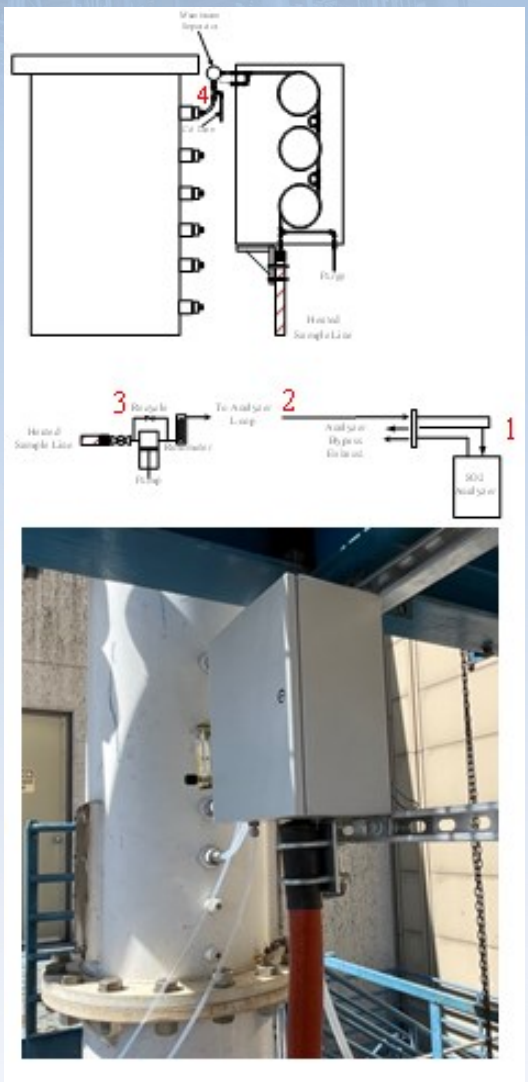
In the pilot study, a 30% piperazine in water solvent will be used to absorb a 4% carbon dioxide from air simulating a flue gas from a natural gas fired boiler. The absorber is configured with three 10-ft beds of RSP250Y structured packing. The bottom two beds are used to absorb carbon dioxide while the upper bed is used in a water wash configuration to scrub volatilized piperazine. The effects of residence time under high temperature conditions, absorber sump residence time, nitrogen stripping within the absorber sump and the low ppm level NO_2 will be studied to determine their effect on solvent oxidation. In addition, carbon adsorption on a solvent slip stream, corrosion and heat loss studies will be incorporated.

In parallel, SRP technicians have been assisting in the commissioning Dr. Rochelle's small pilot scale absorption/stripping system donated by Shell Cansolv. Again a 30% piperazine in water solvent will be used to absorb 4% carbon dioxide from air. The small pilot unit is referred to as the ASAP system will also study solvent oxidation and will operate 24 hours/day five days per week.

A recent packing characterization study has allowed for significantly improved outlet SO2 sampling. A new membrane drier, heated line and refurbished low ppb SO2 analyzer have been tested and found to be very reliable in measuring SO2 concentrations down to 1-2 ppb. The new analytical development will allow measuring gas film volumetric mass transfer coefficients using deeper packed bed heights of 6 to10 ft instead of 1 to 1.5 ft. The analytical enhancement will allow for the collection of improved gas-film controlled performance data using more appropriate bed heights. *cont.* →



The ASAP Pilot System



New Membrane Drier and Heated Sample Line for Outlet SO2 Measurements

SRP Update cont.

SRP oil/water membrane separation studies continue to increase with multiple projects planned in 2021. The studies involve a collaboration with Professors Lynn Katz and Kerry Kinney. A PhD student, Carolyn Cooper, summarized our recent results in our Spring PSTC Meeting. A successful field test was completed in early December 2019 in treating produced water from an Eagle Ford site. The Kuwait Foundation of Science is funding a two-year study. The effects of differing oil concentrations (25-300 pm), oil viscosities, salt concentration, surfactant types and micron and submicron solids handling are planned in 2021/2022. The study includes continued treatment of actual produced water. A new proposal has been submitted to study feeds containing up to 50% oil.

Plans are underway in 2022 to study a novel extractive distillation process related to carbon dioxide emissions reduction. Also, a journal paper is being prepared which will provide SRP performance data related to plastics recycling. Distillation and air/water related packing tests are also planned for early 2022. In addition, a proposal is being prepared to study liquid-liquid-gas separations in a horizontal pilot-scale glass settler.

2022 SRP pilot plant and lab scale operations will include:

- CO2 absorption/stripping pilot campaign focused on improving solvent oxidation
- Gas Film Controlled Spray Mass Transfer
- Distillation Packing Characterization
- Application of near infrared spectrophotometry to Obtain Fast Distillation Compositional Measurements
- Air/Water Packing Characterization
- Oil/Water Membrane Separations

The last year has certainly been challenging, but we managed to conduct an active research program and maintain our staffing levels. This is directly attributed to timely research support, the generosity of the UT Engineering School, and supplemental financial contributions from several of our industrial sponsors. We are very thankful to have weathered the storm and look forward to a more normal 2022.

Presentations

In early September 2022, at the 30th Annual Meeting of the North American Membrane Society (NAMS), several PSTC members from the **Freeman Group** presented papers and posters.

Oral Presentations

- Bridge, Alexander, Benjamin Pedretti, Joan Brennecke, Benny D. Freeman, "Greener Preparation of Defect-Free Asymmetric Gas Separation Membranes with Dihydrolevoglucosenone (CyreneTM) as an Alternative Polar Aprotic Solvent."
- Landsman, Matthew R., Frederick Rivers, Benjamin Pedretti, Gregory Su, Benny D. Freeman, Desmond Lawler, Nathaniel Lynd, and Lynn Katz, "Polyol-Functionalized Polyether Membranes for Selective Removal of Boric Acid."
- Miller, Daniel J., Sergi Molins, Sarah M. Dischinger, Mostafa Nassr, Nicolas Spycher, Nils Tilton, Ji Yeon Lee, William Stringfellow, Jacob Johnston, Pedram Bigdelou, Kristofer Gleason, and Benny D. Freeman, "A Computational and Experimental Test Bed for Prediction of RO Module Fouling."

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Presentations cont.

Oral Presentations cont.

- Oh, Hyeonji, Yu-Ming Tu, Benny D. Freeman, and Manish Kumar, "Membrane Protein (MP) Based Nano-Porous Membranes that Transport Vapor at High Rates while being Impermeable to Water."
- Sujanani, Rahul and Benny D. Freeman, "Revisiting Water and Ion Transport in Nafion."
- Tilton, Nils, Jacob Johnston, Pedram Bigdelou, Sergi Molins, Nicolas Spycher, Sarah M. Dischinger, Mostafa Nassr, Ji Yeon Lee, Kristofer Gleason, William Stringfellow, Benny D. Freeman, and Daniel J. Miller, "Reduced-Order Models of Concentration Polarization in RO Systems with Spacers."
- Tu, Yu-Ming, Hyeonji Oh, Benny D. Freeman, and Manish Kumar, "Membrane Protein-Based Biomimetic Membranes for Water Treatment."
- Zofchak, Everett S., Zidan Zhang, Bill Wheatle, Rahul Sujanani, Sam Warnock, Kalin Hanson, Mahdi Abu-Omar, Chris Bates, Benny D. Freeman, and Venkat Ganesan, "Origins of Cation-Cation Selectivity in Crown Ether-Functionalized Polymer Membranes."

Poster Presentations

- Bigdelou, Pedram, Jacob Johnston, Sarah M. Dischinger, Mostafa Nassr, Ji Yeon Lee, Nils Tilton, Daniel J. Miller, William Stringfellow, Nicolas Spycher, Sergi Molins Rafa, Kristofer Gleason, and Benny D. Freeman, "Reduced-Order Models of Concentration Polarization in Reverse Osmosis Systems with Feed Spacers."
- Bridge, Alexander, Benjamin Pedretti, Joan Brennecke, Benny D. Freeman, "Greener Preparation of Defect-Free Asymmetric Gas Separation Membranes with Dihydrolevoglucosenone (CyreneTM) as an Alternative Polar Aprotic Solvent."
- Johnston, Jacob, Pedram Bigdelou, Sarah M. Dischinger, Mostafa Nassr, Ji Yeon Lee, Nils Tilton, Daniel J. Miller, William Stringfellow, Nicolas Spycher, Sergi Molins Rafa, and Benny D. Freeman, "Computational Fluid Dynamics Simulations of Unsteady Vortex Shedding and Concentration Polarization in Reverse Osmosis Systems."
- Landsman, Matthew R., Frederick Rivers, Benjamin Pedretti, Gregory Su, Benny D. Freeman, Desmond Lawler, Nathaniel Lynd, and Lynn Katz, "Polyol-Functionalized Polyether Membranes for Selective Removal of Boric Acid."
- Oh, Hyeonji, Yu-Ming Tu, Benny D. Freeman, and Manish Kumar, "Membrane Protein (MP) Based Nano-Porous Membranes that Transport Vapor at High Rates while being Impermeable to Water."
- Sujanani, Rahul and Benny D. Freeman, "Revisiting Water and Ion Transport in Nafion."
- Warnock, Sam, Rahul Sujanani, Everett S. Zofchak, Shou Zhao, Theodore Dilenschneider, Kalin Hanson, Sanjoy Mukherjee, Venkat Ganesan, Benny D. Freeman, Mahdi Abu-Omar, and Chris Bates, "Engineering Li/Na Selectivity in 12-Crown-4-Functionalized Polymer Membranes."
- Zofchak, Everett S., Zidan Zhang, Bill Wheatle, Rahul Sujanani, Sam Warnock, Kalin Hanson, Mahdi Abu-Omar, Chris Bates, Benny D. Freeman, and Venkat Ganesan, "Origins of Cation-Cation Selectivity in Crown Ether-Functionalized Polymer Membranes."

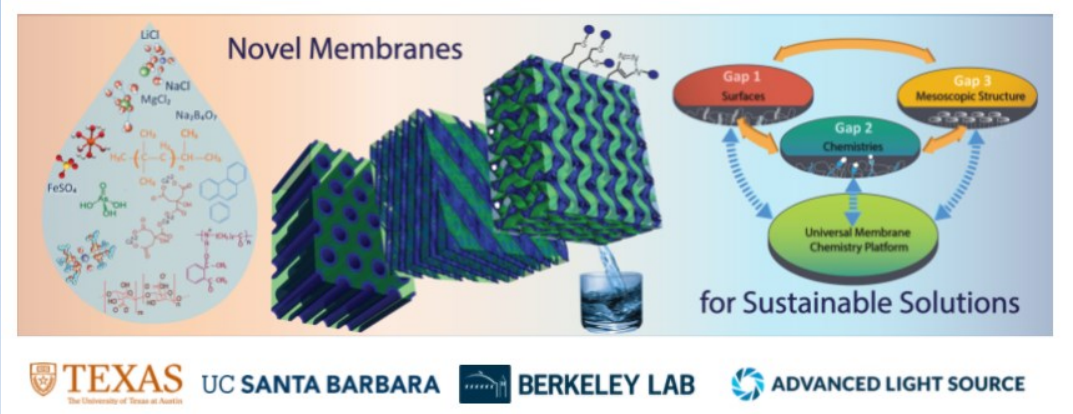
At the upcoming 2022 AIChE Annual Meeting, the following members of the **Freeman**, **Baldea**, and **Seibert Groups** will present their research:

- Tu, Yu-Ming, Benny D. Freeman, and Manish Kumar, "Rapid Self-Assembly: Biomimetic Membranes from Membrane Protein-Block Copolymer Nanosheets."
- Tu, Yu-Ming, Benny D. Feeman, and Manish Kumar, "Membrane Protein-Based Biomimetic Membranes for Water Treatment."
- Santander, Omar and Michael Baldea, "Integrated Planning and Advanced Control of Refining Processes."
- Seo, Kyeongjun and Michael Baldea, "Flexible Operation of Carbon Capture Systems."
- Cooper, Carolyn, Lynn Katz, Kerry Kinney and Frank Seibert, "Oil Recovery from Dilute Oil in Water Mixtures Via Hydrophobic Hollow Fiber Membranes"

In the News

The DOE EFRC Center for Materials for Water and Energy Systems (M-WET), directed by PSTC PI **Benny Freeman** is proud to announce the following awards received by M-WET team members:

- Alec Bridge, graduate student supervised by Professors Freeman and Brennecke, won first place in the North American Membrane Society (NAMS) 2021 Poster Award in Session C: Gas Separation.
- Former graduate student, Jovan Kamcev, now an Assistant Professor at University of Michigan, received the 2021 NAMS Young Membrane Scientist Award. Learn more about his work at https://macro.engin.umich.edu/profile/kamcev-jovan/.
- Varun Hegde, graduate student supervised by Professors Doherty and Squires at UC Santa Barbara), won first place in the North American Membrane Society (NAMS) 2021 Poster Award in Session A: Fundamentals, Emerging Materials, and Processes.
- Akhilesh Paspureddi, graduate Student supervised by Professor Kumar, won the Cockrell School of Engineering Leadership Award. Read more about his award at https://mwet.utexas.edu/news/akhilesh-paspureddi-wins-cockrell-school-engineering-leadership-award.
- Rachel Segalman, Associate Director of M-WET, was elected to the National Academy of Engineering. Learn more about the award at https://mwet.utexas.edu/news/professors-segalman-and-hawker-elected-national-academy-engineering.



Publications

Eldridge Group

- L. Macfarlan, A. F. Seibert, M. T. Phan, R. B. Eldridge. "CFD-based Study on Structured Packing Geometry," *Chem. Eng. Sci.* 243, 116767 (2021).
- M. Walk, J. Hamacher, J. J. Downs, S. M. Miller, S. A. Owens, R. B. Eldridge. "Validation of Differential Temperature Control for Dividing Wall Distillation Column," *Ind. Eng. Chem. Res.*, 60, 1341 (2021).

Freeman Group

- E. Zofchak, Z. Zhang, B. Wheatle, T. Dilenschneider, R. Sujanani, K. Hanson, S. Warnock, S. Zhao, S. Mukherjee, M. Abu-Omar, C. Bates, B. Freeman, and V. Ganesan. "Origins of Lithium/Sodium Reverse Permeability Selectivity in 12-Crown-4-Functionalized Polymer Membranes," *ACS Macro Letters*, in press.
- S. J. Warnock, R. Sujanani, E. S. Zofchak, S. Zhao, T. J. Dilenschneider, K. G. Hanson, S. Mukherjee, V. Ganesan, B.D. Freeman, M.M. Abu-Omar, and C.M. Bates. "Engineering Li/Na Selectivity in 12-Crown-4-functionalized Polymer Membranes," *Proceedings of the National Academy of Sciences (PNAS)*, in press.

cont. →

Publications cont.

Freeman Group cont.

- J. D. Moon, H. Borjigin, R. Liu, R. M. Joseph, J. S. Riffle, B. D. Freeman, D. R. Paul. "Impact of Humidity on Gas Transport in Polybenzimidazole Membranes," *Journal of Membrane Science*, 639, 119758 (2021).
- M. R. Landsman, F. Rivers, B. J. Pedretti, B. D. Freeman, D. F. Lawler, N. A. Lynd, L. E. Katz. "Boric Acid Removal with Polyol-functionalized Polyether Membranes," *Journal of Membrane Science*, 638, 119690 (2021).
- R. Sujanani, L. E. Katz, D. R. Paul, B. D. Freeman. "Aqueous Ion Partitioning in Nafion: Applicability of Manning's Counter-ion Condensation Theory," *Journal of Membrane Science*, 638, 119687 (2021).
- M. Allen, R. Sujanani, A. Chemseddine, B. Freeman, Z. Page. "Mechanically Robust Hydrophobized Double Network Hydrogels and Their Fundamental Salt Transport Properties," *Journal of Polymer Science*, 1 (2021).
- M. Allen, R. Sujanani, A. Chemseddine, B. Freeman, Z. Page. "Mechanically Robust Hydrophobized Double Network Hydrogels for Water Purification," *ChemRxiv* (2021).
- Y. Yu, N. Yan, B.D. Freeman, C.-C. Chen. "Mobile Ion Partitioning in Ion Exchange Membranes Immersed in Saline Solutions," *Journal of Membrane Science*, **620**, 118760 (2021).
- A. L. P. Nguyen, T. G. Mason, B. D. Freeman, E.I. Izgorodina. "Prediction of Lattice Energy of Benzene Crystals: A Robust Theoretical Approach," *Journal of Computational Chemistry*, **42**, 248-260 (2021).
- J. D. Moon, R. Sujanani, Z. Geng, B. D. Freeman, R. A. Segalman, C. J. Hawker. "Versatile Synthetic Platform for Polymer Membrane Libraries Using Functional Networks," *Macromolecules*, **54**(2), 866-873 (2021).
- J. Park, H. Ha, H. W. Yoon, J. Noh, H. B. Park, D. R. Paul, C. J. Ellison, B. D. Freeman. *"*Gas Sorption and Diffusion in Poly(dimethylsiloxane) (PDMS)/Graphene Oxide (GO) Nanocomposite Membranes*," Polymer,* **212**, 123185 (2021).
- C. Soto, E. S. Torres-Cuevas, A. González-Ortega, L. Palacio, Á. E. Lozano, B. D. Freeman, P. Prádanos. "Gas Separation by Mixed Matrix Membranes with Porous Organic Polymer Inclusions within *o*-Hydroxypolyamides Containing *m*-Terphenyl Moieties," *Polymers*, **13**(6), 931 (2021).

Fall 2021 Meeting

Please join us for our annual PSTC Fall Meeting, scheduled for Tuesday, October 19, and Wednesday, October 20, 2021, occurring online via Zoom. Please stay tuned to https://sites.utexas.edu/pstc/conferences/ for more infor-

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