

James R. Fair Process Science & Technology Center



Spring 2021 Newsletter

Note from the Program Head

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

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I want to thank everyone who took the opportunity to participate in the Spring 2021 PSTC meeting. As I said earlier, the ability to hold the meeting virtually and make the presentation recordings available to our sponsors has been a positive take-away from the pandemic. I thought the student presentations were outstanding this meeting, and were certainly a testimony to the quality of the students attracted to the type of research our PI's conduct.

The center continues to do well despite the challenging times. Our cash flow is still relatively strong with the pilot plant experimental program seeing the most negative impact over the past year. We were in discussions with the Engineering Dean's office about the pilot plant steam system piping replacement at the time the first cases were reported last year. As you might guess, even before the damage associated with the low temperatures in February, cash had become relatively tight. My guess is we will need to come up with some cost share money in order to get funds from the dean. The piping replacement is critical if we are going to keep the pilot plant running.

As most of you know, in my other job I teach in the Chemical Engineering Department and several of you have asked about my experience with on-line course offerings. I have been fortunate to be teaching the senior design course all three long semesters along with the separations processes course last summer. All four courses are populated with junior and senior stu-

dents who are house broken which probably makes the switch to on-line instruction easier than a freshman / sophomore course. We have been doing the course, recitation, and office hours via ZOOM. I have tried to make the students' experience as close to the in-class model as possible which might be a slight departure from what you hear being proposed as the best plan. I assumed the students had enough disruption and that changing the course methodology was one they did not need to suffer through – class teaching evaluations for various approaches supported this assumption.

On balance the on-line approach has worked pretty well; the students are learning the material probably as well as the in-class approach with last fall's design reports as good as any I have received. I have increased my office hour flexibility; last April the design class had several students who had gone home to China which made for interesting 10:00 pm design group sessions. One short-coming of the on-line environment is the inability to maintain test integrity. There are software packages which will "watch" students take exams but none of them are applicable for the pencil on paper exams we give. I have gotten to a happy place with never being totally sure the work is uncompromised.

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Program Head Note Cont.

I also switched the separations course exams to take -home projects instead of “in class” exams. Having said all this, teaching on-line is just not a lot of fun for anybody. I miss the student interaction both inside and outside of class and I am sure the students miss the group learning environment of the McKetta study hall. We are all looking forward to next fall when things return to whatever passes for

“normal” post-pandemic.

Best wishes and please contact me anytime with questions or concerns. I am looking forward to visiting with you face-to-face at the fall PSTC meeting.

Bruce

SRP Update: Frank Seibert



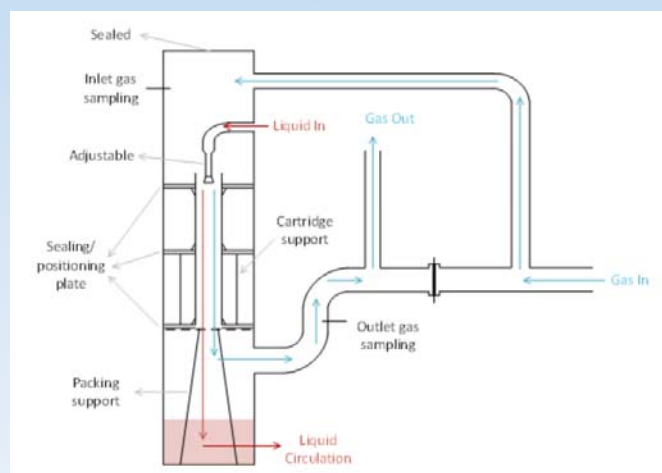
The SRP pilot remains active with several studies completed, underway or in the planning stages. In mid-February, Texas, including Austin, suffered a severe and prolonged freeze event where electrical power was out for more than a week in many locations. My office and especially my home experi-

enced significant freeze damage. Fortunately, it appears the pilot plant survived the freeze with very minor damage which has been corrected. Our interior building temperature dropped well below freezing which caused extensive damage to our building's utility room which resulted in flooding of some offices. Fortunately, our labs did not experience flood damage.

Three distillation packing performance studies were recently completed and summarized in the Spring PSTC Meeting. RVT Process Equipment GmbH recently studies of a new high performance random packing referred to as RMXR#2. The packing provided similar mass transfer performance with the 2-inch Pall Ring but with 30% additional capacity. Distillation under severe corrosive conditions and high temperature may require the use of very exotic metallurgy. The SRP has often been asked about ceramic structured packings. With the support of RVT, two ceramic structured packings referred to as RVT RCP S250 were studied using the standard cyclohexane/n-heptane test system. The effects of a glazed and unglazed surface were determined. The performance results were also summarized in our Spring PSTC SRP Update Presentation. The random and ceramic structured packing data have been added to the SRP Packing Database.

Co-current gas film mass transfer controlled spray studies have been performed which include a significant amount of experimental variations. It is noted that such data do not exist in the published literature. The study required modifying our air/water column to allow for co-current contacting. The Air/SO₂/0.1 N NaOH test system is used in these gas film mass transfer controlled studies. Limited runs also include the Air/SO₂/Sodium Carbonate system. Three spray nozzle types (Full Cone, Flat Cone and Hollow Cone) and various contacting heights were studied. In addition, the effect of contacting height and an empty column were determined.

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Modified Air/Water Column for Co-Current Spray Studies

SRP Update cont.

The interesting results were summarized in our Spring PSTC presentation. The mass transfer efficiency with spray nozzles was found to be very dependent on the contacting length. The results indicated a large fraction of the mass transfer occurs in the vicinity of the spray nozzle. Nevertheless as shown in the empty column study, mass transfer also occurs along the wall.

A recent study has allowed for improved outlet SO_2 sampling. A new membrane drier, heated line and refurbished low ppb SO_2 analyzer have been tested and found to be very reliable in measuring SO_2 concentrations down to 2 ppb. The new analytical development will allow measuring gas film volumetric mass transfer coefficients using deeper packed bed heights (2X-2.5X).

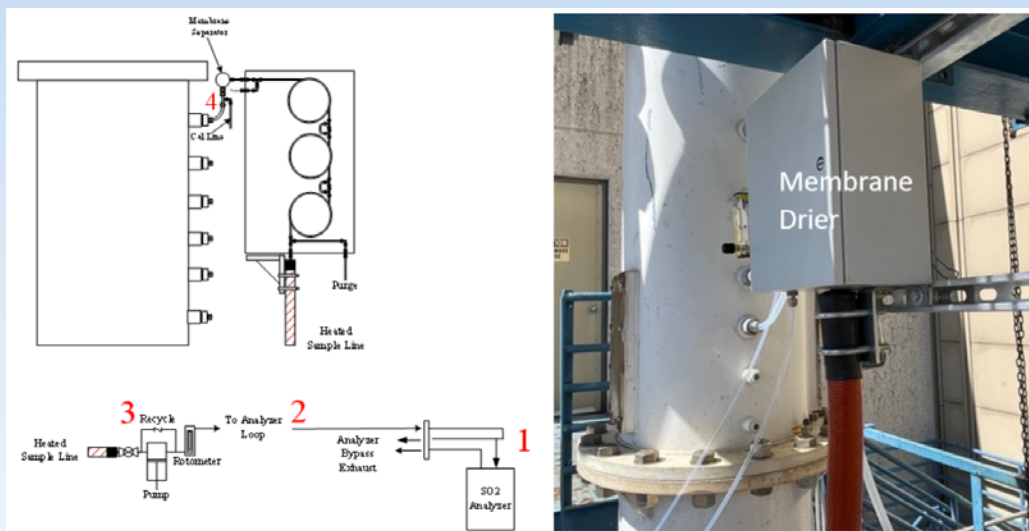
The capacity of a liquid-liquid extractor can be limited by poor drop coalescence at the main operating interface. This is especially true for many “wash” type extractors. In the 1990s, an SRP study was conducted to investigate the performance of Teflon and stainless structured packings in enhancing coalescence and increasing extractor capacity. In some cases, the coalescer addition increased the capacity by 60%. In recent years, new questions regarding coalescer designs have emerged which suggest that a larger study is needed. Such questions include:

- ◆ Can Teflon random packing provide a cost efficient alternative to Teflon structured packing?
- ◆ Are less expensive polypropylene packings as efficient as Teflon packings?
- ◆ What coalescer height is recommended?
- ◆ What capacity increase should be expected with a coalescer addition?
- ◆ What coalescer material of construction should be specified?

Many other related questions have been raised in the last ten years. Prior to COVID, several PSTC sponsors proposed forming a group of PSTC sponsors to provide technical guidance and leveraging of Tier II level funds to support this study. We will be contact with these sponsors to determine if interest is still present and if financial support is possible in 2022.

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 three-year study.

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New Membrane Drier and Heated Sample Line for Outlet SO_2 Measurements

SRP Update cont.

The effects of differing oil concentrations (25-300 pm), surfactant types and micron and submicron solids handling are planned in 2021. The study includes continued treatment with actual produced water. A new proposal has been submitted to study feeds containing up to 50% oil.

Plans are underway to prepare for a 2021 pilot scale carbon dioxide absorption/stripping project. SRP personnel will help support Gary Rochelle's planned studies. A number of piping and equipment modifications will be required. In addition, SRP technicians have been assisting in trouble-shooting and commissioning of donated absorption/stripping lab scale system.

2021 SRP pilot plant and lab scale operations will include:

- ◆ Gas Film Controlled Spray Mass Transfer
- ◆ Distillation Packing Characterization of Unique Structures
- ◆ Application of NIR to Obtain Fast Distillation Compositional Measurements
- ◆ Air/Water Packing Characterization
- ◆ Oil/Water Membrane Separations
- ◆ Pilot Scale CO₂ Absorption/Stripping Preparations

We have been very fortunate in obtaining industrial project funding especially in early days of the COVID shutdown. We sincerely thank our 2020 and 2021 project sponsors. As a reminder, we receive little or no State or Federal support. All of our funding for salaries and equipment maintenance come from industrial-supported projects. We are in need of projects for the second half of 2021. If interested, please contact me at fseibert@mail.utexas.edu or 512/471-7063.



In the News

- ◆ Lingqing Yan of the Baldea/Edgar Group, successfully defended her thesis and will be joining Alibaba Cloud in Hangzhou, China, in August. Congratulations, Lingqing!
- ◆ Morgan Kelley and Fernando Lejarza of the Baldea Group received First and Second Place in the UT Energy Week student research competition! The presentations can be viewed here on UT Energy Week's website: <https://energyweek.utexas.edu/longhorn-energy-club-student-research-competition/>.



Publications

Baldea Group

- ♦ O. Nordness, P. Kelkar, Y. Lyu, M. Baldea, M. A. Stadtherr, J. F. Brennecke. “Predicting Thermo-physical Properties of Dialkylimidazolium Ionic Liquids from Sigma Profiles, *J. Molecular Liquids*, 334, 116019 (2021). <https://doi.org/10.1016/j.molliq.2021.116019>
- ♦ L. Yan, T. F. Edgar, M. Baldea. “Dynamic Process Intensification: Fundamentals and Implementation to Ternary Distillation,” *AIChE J.* (2021). <https://dx.doi.org/10.1002/aic.17262>
- ♦ K. Seo, C. Tsay, T.F. Edgar, M.A. Stadtherr, M. Baldea. “Economic Optimization of Carbon Capture Processes Using Ionic Liquids: Flexibility in Capture Rate and Feed Composition,” *ACS Sus. Chem. Eng.* (2021). <https://dx.doi.org/10.1021/acssuschemeng.1c00066>.
- ♦ J. G. Costandy, T. F. Edgar, M. Baldea. “Elucidating Batch vs. Continuous-Flow Configurations: A Unified Framework for Reactor Network Synthesis,” *Ind. Eng. Chem. Res.*, accepted
- ♦ L. Yan, P. M. Witt, T. F. Edgar, M. Baldea. “Static and Dynamic Intensification of Water-Ethylene Glycol Separation using a Dividing Wall Column,” *Ind. Eng. Chem. Res.*, 60(7), 3027-3037 (2021). <https://dx.doi.org/10.1021/acs.iecr.0c06139>
- ♦ J. I. Otashu, K. Seo, M. Baldea. “Cooperative Optimal Power Flow with Flexible Chemical Process Loads,” *AIChE J.*, 67(4), e17159 (2021). <https://doi.org/10.1002/aic.17159>
- ♦ F. Y. Lee, T. F. Edgar, M. Baldea, J. Lee. “Shape Factor for the Relay Feedback Autotuning,” *The Indian Chemical Engineer* (2020). <https://doi.org/10.1080/00194506.2020.1846630>
- ♦ F. Lejarza, M. Baldea. “Economic Model Predictive Control for Robust Optimal Operation of Sparse Storage Networks, *Automatica* 125, 109346 (2021). <https://doi.org/10.1016/j.automatica.2020.109346>

Eldridge Group

- ♦ M. Walk, J. Hamacher, J. J. Downs, S. M. Miller, S. Owens, R. B. Eldridge. “Validation of Differential Temperature Control for a Dividing Wall Distillation Column,” *Ind. Eng. Chem. Res.* 60, 3, 1341–1355 (2021). <https://pubs.acs.org/doi/abs/10.1021/acs.iecr.0c04570>

Freeman Group

- ♦ Y. Yu, N. Yan, B. D. Freeman, C.-C. Chen, “Mobile Ion Partitioning in Ion Exchange Membranes Immersed in Saline Solutions,” *J. Mem. Sci.*, 620, 118760 (2021). <https://doi.org/10.1016/j.memsci.2020.118760>

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Publications cont.

Freeman Group cont.

- ♦ 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). <https://doi.org/10.1016/j.polymer.2020.123185>
- ♦ 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(4), 248-260 (24 November 2020). <https://doi.org/10.1002/jcc.26452>
- ♦ E. Zofchak, B. Wheatie, Z. Zhang, B. Freeman, V. Ganesan, "Origins of Permselectivity in Lithium/Sodium Reverse-Selective 12-crown-4 Ether Functionalized Polymer Membranes," *Bulletin of the American Physical Society* (15 March 2021). [APS March Meeting 2021]

Fall 2021 Meeting

Please join us for our annual PSTC Fall Meeting, scheduled for Tuesday, October 19, and Wednesday, October 20, 2021, occurring both in person at UT Austin's main campus and online. Please stay tuned to <https://sites.utexas.edu/pstc/conferences/> for more information.

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