

James R. Fair Process Science & Technology Center



Fall 2020 Newsletter

Note from the Program Head

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



Greetings from the home of-
fice from
which I have
taught the sec-
ond half of the
spring senior
design course,
the separations
processes

course during the first summer ses-
sion, and two weeks of the fall senior
design course. I can safely say, while
we are doing OK and the on-line in-
struction is being relatively well re-
ceived by the students, it is not nearly
as much fun. I am guessing this pret-
ty much sums up everyone's experi-
ence since March. We continue to
effectively run research activities on
the main campus and at Pickle using
an innovative cohort approach which
manages the flow of researchers in
and out of the facilities. So far, so
good, with no major outbreaks of
Covid-19 (we are currently doing sig-
nificantly better than Major League
Baseball). Speaking of sports, UT
announced significant layoffs and sal-
ary reductions in the athletic depart-
ment effective September 1st. I
would assume all my corporate part-
ners are seeing the same scenario play
out. The PSTC / SRP is doing rela-
tively well but we are concerned
about cash flow as we move into
2021. The PSTC fortunately was in
the second year of a two-year contract
period in 2020 which provided a
cushion against the pandemic-induced
downturn. This will not be the case in
2021 with renewal contracts for the
next two-year period being due Janu-
ary 1, 2021. I would ask that my cor-

porate colleagues read the tea leaves
and give me a sense of renewal issues
prior to the first of October. Lauren
will send out 2021 / 2022 renewal
contracts around the middle of Octo-
ber. I will be more than happy to dis-
cuss the program at any time with an-
yone, so please contact me. I am bi-
ased, but I truly believe the benefits
of the program continue to be relevant
even in a severe economic downturn.
Unless we intend to turn off the lights
and go home, well-trained students
and applicable forward-thinking re-
search will be required to drive tech-
nology advancement. These are two
items the PSTC and SRP has supplied
to our sponsors for over 35 years.

The fall PSTC meeting will be held
on Tuesday, October 13th. Our virtu-
al meeting platform is ZOOM so
please let me know if this will cause
issues with your corporate firewalls,
etc. A benefit of ZOOM is cloud re-
cording which I have used effectively
in class. As an aside, I actually had
three students this summer who
worked full-time jobs, watched the
lectures later in the day, and still did
very well in the course. The recorded
meeting will benefit our sponsors in
Europe and Asia and anyone interest-
ed in viewing the presentations at a
later date.

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

Best wishes and stay safe,

Bruce

In This Issue:

SRP Update	2
In the News	3
Student Spotlight	4
Publications	6
Fall Meeting	8

SRP Update: Frank Seibert

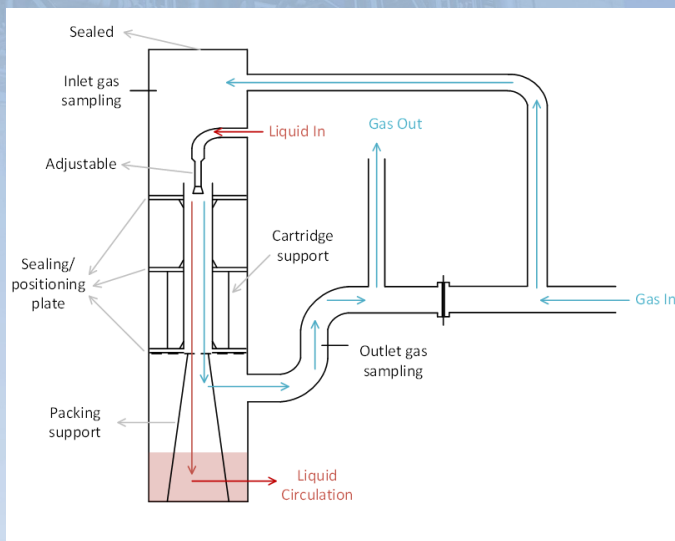


The SRP pilot studies are continuing while managing with the coronavirus related limitations. Several studies are underway.

Since March, lab and pilot scale activities have focused on distillation separations involving pine oil and the recovery of high purity (>98%) α -pinene, β -pinene, and α -terpineol. α -Pinene and β -Pinene are established anti-viral, anti-fungal and anti-microbial chemicals in the medicinal field. There are numerous NIH papers addressing their effectiveness. These chemicals are very effective cleaning and disinfecting agents. The pure chemical samples are needed by two Minnesota labs to determine their viability in killing several pathogens including *Klebsiella Pneumoniae* and *Staphylococcus Aureus* (MRSA), *Pseudomonas Enterica*, Hepadnaviruses (Hepatitis B), and Severe Acute Respiratory Syndrome (SARS CoV-2 Coronavirus that causes COVID-19 disease). The applications will cover the uses for fabric cleaning and hard surface disinfection for Non-food Contact Sanitizers,



water-soluble powders/liquids, and spray products. These chemicals will also be used to treat agricultural diseases affecting the US citrus and Italian olive industries. These studies are being supported by T&R Chemicals. For the first time in its 34 year history, the SRP pilot distillation column is being used to perform batch distillations. These studies will provide interesting data comparing a 40 tray Oldershaw column with a 16.8 inch diameter column filled with two beds of gauze structured packing.



Modified Air/Water Column for Co-Current Spray Studies

Resuming in May, co-current gas film mass transfer controlled spray studies have been performed which include a significant amount of experimental variations. The study utilizes a modification of the 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 have been studied.

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. *cont.* →

SRP Update cont.

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. Several PSTC sponsors have recently proposed that we explore the possibility of forming a group of PSTC sponsors which provide technical guidance and leveraging of their Tier II funds to support this study.

Interest in the SRP oil/water membrane separations process continues to increase with multiple projects planned in 2020. The studies involve a collaboration with Professors Lynn Katz and Kerry Kinney. A PhD student, Carolyn Cooper, is also participat-

ing in these studies. A successful field test was completed in early December in treating produced water from an Eagle Ford site. The Kuwait Foundation of Science is funding a three-year study. The effects of differing oil concentrations (25-200 pm), surfactant types and micron and submicron solids handling are planned in the study. The study includes continued treatment of actual produced water.

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.

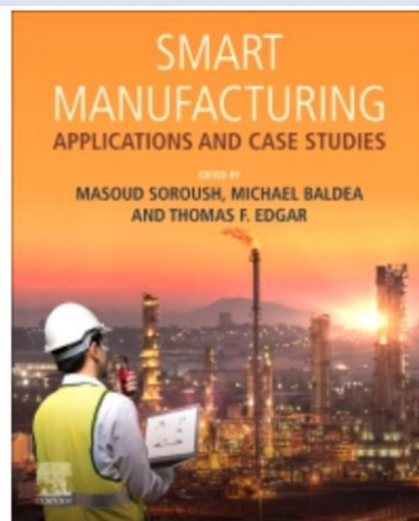
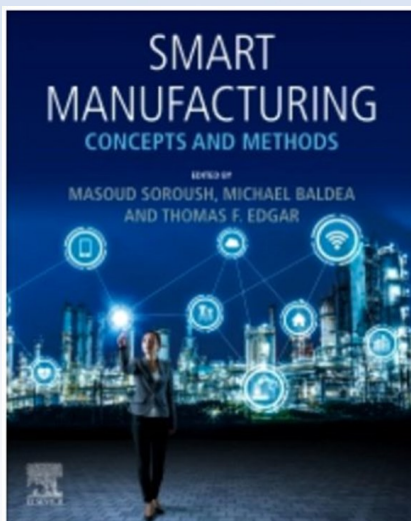
2020-2021 SRP pilot plant and lab scale operations will include:

- ◆ 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
- ◆ Batch Distillation to Obtain High Purity Chemicals from Pine Oil Feedstocks
- ◆ Pilot Scale CO₂ Absorption/Stripping Preparations

In the News

Smart Manufacturing

UT professors **Michael Baldea** and **Thomas Edgar** are excited to announce the publication of their two (co-authored with Professor Masoud Soroush from Drexel University): [*Smart Manufacturing: Concepts and Methods*](#) and [*Smart Manufacturing: Applications and Case Studies*](#). These books comprehensively cover research advances and key applications of smart manufacturing to date. These books are available directly from Elsevier or from your favorite bookseller.



In the News cont.

El-Halwagi Receives AIChE Award



Professor **Mahmoud El-Halwagi** of Texas A&M University has received the 2020 Computing in Chemical Engineering Award from the American Institute of Chemical Engineers. Dr. El-Halwagi is the Managing Director of the Gas and Fuels Research Center at Texas A&M and focuses his research on sustainability, process integration, synthesis, design, operation, and optimization. [Read the full announcement here on the AIChE website!](#)

Freeman & Collaborators Conduct Ground-Breaking Research



Professor **Benny Freeman** of the University of Texas at Austin is at the leading edge of innovative research. The US Army has awarded UT Austin funding as part of the Department of Defense's [Multidisciplinary University Research Initiative \(MURI\)](#) program. Taking inspiration from a small insect, the leafhopper, the group aims to understand how the leafhopper produces a substance that makes it water-repellant

and anti-reflective and work towards producing synthetic options. These synthesized products could have applications in a variety of materials including camouflage and water purification. [Read the full article here on UT Austin's College of Natural Sciences website.](#)

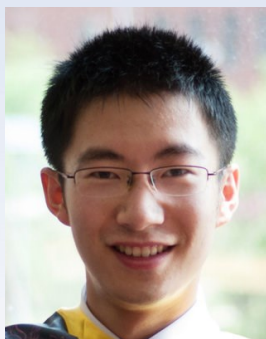
An international research team, **Freeman** among them, have created a new filtration technique that reduces lithium extraction from the earth, shortening the process from years and months down to just hours. The team developed a Metal-Organic Framework channel membrane that filters lithium through a fast, one-directional, highly selective membrane. This new technique could benefit not only renewable energy-based technology (such as electric cars) but also Freeman's focus on low-energy water purification. Read more about this [pioneering technique here on UT Austin's Cockrell School of Engineering website](#) and in the [group-authored publication in Nature Materials.](#)



Student Spotlight: Tianyu Gao

In this issue of our Student Spotlight, **Tianyu Gao**, a graduate research assistant in chemical engineering in the **Rochelle Group**, introduces himself to us and shares his background, his experiences, and his goals.

Tianyu Gao: "I was born in Hefei, east China. By the time I was in middle school, I had a great interest in exploring the universe and had a dream of becoming an astronaut. Later, my fascination with the great universe transferred to exploring the universal rules of physics and chemistry and motivated me to study science and engineering.



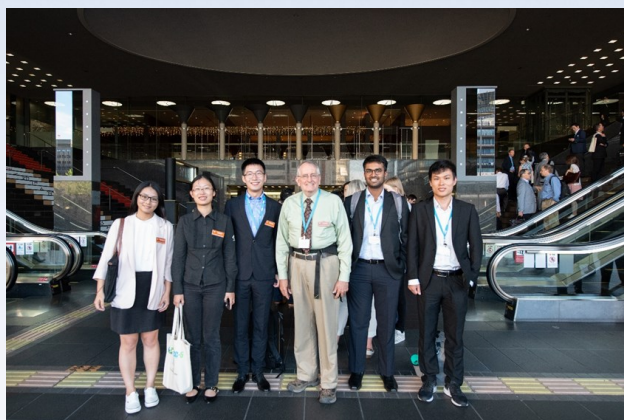
Moving to Dalian and attending Dalian University of Technology, I decided to study chemical engineering because I was interested in chemistry and was impressed by the great achievements made by engineers that improve our life dramatically. I was introduced to the process during the course of plant design. I was excited about applying the fundamental knowledge I learnt from classes into designing of a plant and solving practical problems.

cont. →

Student Spotlight cont.

Driven by the passion and determination to make an impact in chemical engineering, I sought out opportunities to graduate studies and to do independent research. I went Carnegie Mellon University in Pittsburgh and obtained my masters' degree. Having a chance to apply theoretical knowledge to real engineering problems is fantastic, and this is even more appealing after getting to know computational methods during my master's study. At CMU where intelligence cooperates with computers, I realized the rapid advancement in computational tools and the dramatic methodology changes happening to chemical engineering.

After finishing my master's degree, I decided to continue research and applying my expertise to solving practical engineering problems. I joined Dr. Rochelle's research group and PSTC at the University of Texas, conducted research in CO₂ capture area, and solved practical engineering problem. My research project focuses on the simulating and understanding of the system performance, validating with pilot plant experiments, and optimizing the carbon capture process. By working with the large amount of data from pilot plant experiments, I accumulated valuable experience on data analysis and uncertainty quantification. With the validated process model, I also designed and optimized the flue gas pretreatment, absorber column, and water wash system of a commercial-scale amine scrubbing plant for a Front-End Engineering Design study. With the collaboration with engineering companies and experienced engineers, I managed to solve a practical problem, design the system, and demonstrate the technical feasibility.



The Rochelle Group at Kyoto for the Post-combustion Carbon Capture 5.

As part of my graduate study, I also joined Electric Power Research Institute (EPRI) for a summer internship. I was working on a project to evaluate the capture cost for high CO₂ capture rate. I was able to work with the team that has great experience in the research of carbon capture as well as the connection with industry. Although the internship was in the form of remote participation because of the pandemic, it still provided me with the opportunities to conduct impactful research, to have a broader view of carbon capture, and to connect with industry.

From my perspective, the biggest challenge facing by the energy industry is the transition to systems and technologies that simultaneously address the most fundamental needs—energy security, economic competitiveness, and the increasing environmental responsibility. Reducing CO₂ emission has become an urgent request to address the global warming. This provides the opportunity for large-scale deployment of Carbon Capture and Storage technologies. I am glad that I chose CO₂ capture as my research area and made my contribution to the technology advance. I hope to continue to work on the energy industry after graduation and pursue a more sustainable and environmental-friendly pathway.

In my leisure time, I enjoy outdoor activities and photography. I like visiting national park, camping, shooting landscape and wildlife photos.”

The Rochelle Group and the Process Science & Technology Center are proud to have Tianyu Gao as an active and passionate member of our research team!



Tianyu at the National Carbon Capture Center

Publications

El-Halwagi Group

- ♦ H. Baaqeel, A. Alghamdi, F. Abdelhady, and M. M. El-Halwagi, "Optimal Design and Scheduling of a Solar-Assisted Domestic Desalination Systems," *Comp. Chem. Eng.* **132**, 106605 (2020). <https://doi.org/10.1016/j.compchemeng.2019.106605>
- ♦ R. Mukherjee, R. R. Asani, N. Boppana, and M. M. El-Halwagi, "Performance Evaluation of Shale Gas Processing and NGL Recovery Plant under Uncertainty of the Feed Composition," *Journal of Natural Gas Science & Engineering* (in press). <https://doi.org/10.1016/j.jngse.2020.103517>
- ♦ A. Al-Douri, V. Kazantzi, F. T. Eljack, and M. M. El-Halwagi, "Mitigation of Operational Failures via an Economic Framework of Reliability, Availability, and Maintainability (RAM) During Conceptual Design," *Journal of Loss Prevention in the Process Industries* (in press). <https://doi.org/10.1016/j.jlp.2020.104261>
- ♦ K. Cao, P. Siddhamshetty, Y. Ahn, M. M. El-Halwagi, and J. S. I. Kwon, "Evaluating the Spatiotemporal Variability of Water Recovery Ratios of Shale Gas Wells and Their Effects on Shale Gas Development," *Journal of Cleaner Production*, 123171 (2020). <https://doi.org/10.1016/j.jclepro.2020.123171>
- ♦ D. Oke, R. Mukherjee, D. Sengupta, T. Majozzi, and M. M. El-Halwagi, "Hybrid Regeneration Network for Flowback Water Management," *Industrial & Engineering Chemistry Research* (2020). <https://doi.org/10.1021/acs.iecr.0c01361>
- ♦ S. I. Meramo-Hurtado, E. Sanchez-Tuiran, J. M. Ponce-Ortega, M. M. El-Halwagi, and K. A. Ojeda-Delgado, "Synthesis and Sustainability Evaluation of a Lignocellulosic Multifeedstock Biorefinery Considering Technical Performance Indicators," *ACS Omega*, 5(16), 9259-9275 (2020). <https://doi.org/10.1021/acsomega.0c00114>
- ♦ O. Abdelaziz, A. Al-Rabiah, M. M. El-Halwagi, and C. Hulteberg, "Conceptual Design of a Kraft Lignin Biorefinery for the Production of Valuable Chemicals via Oxidative Depolymerization," *ACS Sustainable Chemistry and Engineering* (in press, 2020).
- ♦ M. Wang, C. Deng, H. Chen, X. Wang, B. Liu, C. Sun, G. Chen, and M. M. El-Halwagi, "An Analytical Investigation on the Energy Efficiency of Integration of Natural Gas Hydrate Exploitation with H₂ Production (by in-situ CH₄ Reforming) and CO₂ Sequestration," *Energy Conversion and Management*, 216, 112959 (2020). <https://doi.org/10.1016/j.enconman.2020.112959>
- ♦ D. Oke, R. Mukherjee, D. Sengupta, T. Majozia, and M. M. El-Halwagi, "On the Optimization of Water-Energy Nexus in Shale Gas Network under Price Uncertainties," *Energy*, 117770 (2020). <https://doi.org/10.1016/j.energy.2020.117770>
- ♦ S. Park, S. Xu, W. Rogers, H. Pisman, and M. M. El-Halwagi, "Incorporating Inherent Safety during the Conceptual Process Design Stage: A Literature Review," *Journal of Loss Prevention in the Process Industries*, 63, 104040 (2020). <https://doi.org/10.1016/j.jlp.2019.104040>

cont. →

Publications cont.

El-Halwagi Group cont.

- ♦ L. G. Hernández-Pérez, A. S. Alsuhaibani, N. Radwan, M. M. El-Halwagi, and J. M. Ponce-Ortega, "Structural and Operating Optimization of the Methanol Process Using a Metaheuristic Technique," *ACS Sustainable Chemistry & Engineering*, 8, 3135-3150 (2020). <https://doi.org/10.1021/acssuschemeng.9b05981>
- ♦ Y. Xu, H. Dinh, Q. Xu., F. T. Eljack, and M. M. El-Halwagi, "Flare Minimization for An Olefin Plant Shutdown via Plant-wide Dynamic Simulation," *J. Cleaner Production*, 254, 120129 (2020). <https://doi.org/10.1016/j.jclepro.2020.120129>

Freeman Group

- ♦ M. Galizia, D. R. Paul, and B. D. Freeman, "Co-ion Specific Effect on Sodium Halides Sorption and Transport in a Cross-linked Poly(p-styrene sulfonate-co-divinylbenzene) for Membrane Applications," *Journal of Membrane Science*, 612, 118410 (2020). <https://doi.org/10.1016/j.memsci.2020.118410>
- ♦ J. D. Moon, B. D. Freeman, C. J. Hawker, and R. A. Segalman, "Can Self-Assembly Address the Permeability/Selectivity Trade-Off in Polymer Membranes," *Macromolecules*, 53(14), 5649-5654 (2020). <https://doi.org/10.1021/acs.macromol.0c01111>
- ♦ J. F. Brennecke and B. D. Freeman, "Reimagining Petroleum Refining," *Science*, 369(6501), 254-255 (July 2020). <https://doi.org/10.1126/science.abd1307>
- ♦ M. R. Landsman, R. Sujanani, S. H. Brodfuehrer, C. M. Cooper, A. G. Darr, R. J. Davis, K. Kim, S. Kum, L. K. Nalley, S. M. Nomaan, C. P. Oden, A. Paspureddi, K. K. Reimund, L. S. Rowles III, S. Yeo, D. F. Lawler, B. D. Freeman, and L. E. Katz, "Water Treatment: Are Membranes the Panacea?" *Annual Review of Chemical and Biomolecular Engineering*, 11, 559-585 (2020). <https://doi.org/10.1146/annurev-chembioeng-111919-091940>
- ♦ G. Q. Chen, K. Wei, A. Hassanvand, B. D. Freeman, and S. E. Kentish, "Single and Binary Ion Sorption Equilibria of Monovalent and Divalent Ions in Commercial Ion Exchange Membranes," *Water Research*, 175, 115681 (2020). <https://doi.org/10.1016/j.watres.2020.115681>
- ♦ E.-S. Jang, J. Kamcev, K. Kobayashi, N. Yan, R. Sujanani, T. J. Dilenschneider, H. B. Park, D. R. Paul, and B. D. Freeman, "Influence of Water Content on Alkali Metal Chloride Transport in Cross-linked Poly(ethylene glycol) Diacrylate. 2. Ion Diffusion," *Polymer*, 192, 122316 (2020). <https://doi.org/10.1016/j.polymer.2020.122316>
- ♦ J. Lu, H. Zhang, J. Hou, X. Li, X. Hu, Y. Hu, C. D. Easton, Q. Li, C. Sun, A. W. Thornton, M. R. Hill, X. Zhang, G. Jiang, J. Z. Liu, A. J. Hill, B. D. Freeman, L. Jiang, and H. Wang, "Efficient Metal Ion Sieving in Rectifying Subnanochannels Enabled by Metal-Organic Frameworks," *Nature Materials*, (2020). <https://doi.org/10.1038/s41563-020-0634-7>
- ♦ J. Park, H. W. Yoon, D. R. Paul, and B. D. Freeman, "Gas Transport Properties of PDMS-coated Reverse Osmosis Membranes," *Journal of Membrane Science*, 604:118009 (2020). <https://doi.org/10.1016/j.memsci.2020.118009>

cont. →

Publications cont.***Freeman Group cont.***

- ◆ H. W. Yoon, C. M. Doherty, T. H. Lee, T. H. Choi, J. S. Roh, H. W. Kim, Y. H. Cho, S.-H. Do, B. D. Freeman, and H. B. Park, "Origin of CO₂-philic Sorption of Graphene Oxide Layered Nanosheets and Its Derivatives," *J. Phys. Chem. Lett.*, 11(6), 2356-2362 (2020). <https://doi.org/10.1021/acs.jpcltt.0c00204>
- ◆ C. Miguel Sanchez, T. Song, J. Brennecke, and B. Freeman, "Hydrogen Stable Supported Ionic Liquid Membranes with Silver Carriers: Propylene and Propane Permeability and Solubility," *Industrial & Engineering Chemistry Research*, 59(12), 5362-5370 (2019). <https://doi.org/10.1021/acs.iecr.9b04886>

Fall 2020 Meeting

Please join us for our annual PSTC Fall Meeting, scheduled for Tuesday, October 13, 2020, occurring via Zoom. Please stay tuned to <https://sites.utexas.edu/pstc/conferences/> for more information.

Process Science & Technology Center

University of Texas at Austin
Building 133, Suite 1.312
10100 Burnet Rd., Mail Code R7100
Austin, TX 78758

(p) (512) 471-7077
lauren.murrah@austin.utexas.edu
<https://sites.utexas.edu/pstc/>

