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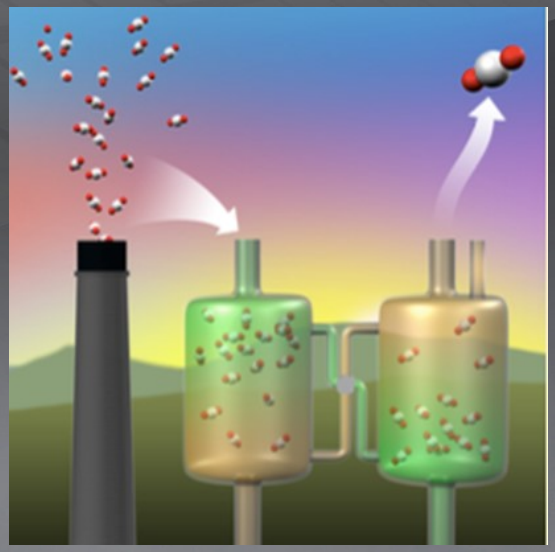

Low-Viscosity, Water-Lean CO_2BOLs with Polarity-Swing Assisted Regeneration (FWP-70924)

Richard Zheng (for David Heldebrant)

2019 Carbon Capture, Utilization, Storage, and Oil & Gas Technologies Integrated Review Meeting
Pittsburgh, PA August 28, 2019

DOE/NETL Federal Project Manager: Sai Gollakota

Acknowledgment

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Project Objectives

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Solvent R&D that accelerates the development of post-combustion technologies that may impact the broader solvent community.

- Follow the model for DOE's Discovery of Carbon Capture Substances and Systems (DOCCSS) Initiative: leverage national labs and industry to rapidly scale-up and demonstrate transformational capture technologies.
- Focus on a promising 3rd Generation CO_2BOL solvent candidate from prior PNNL solvent development work.
- Engage a powerful industry team – RTI, EPRI, and Fluor Corporation.
- Leverage the capabilities in the Carbon Capture Simulation for Industry Impact ($CCSI^2$) program.
- Demonstrate the technology on a slip stream system.

Integrated R&D Approach

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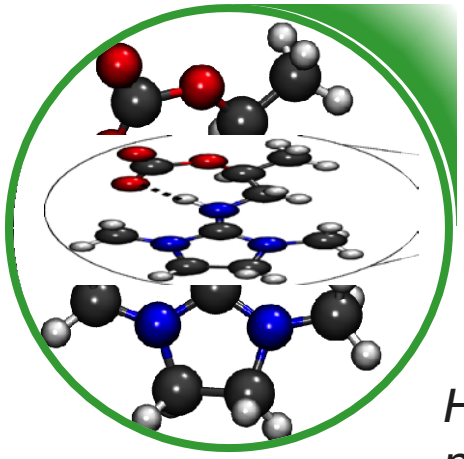
- Solvent Molecular Design
- Property Predictions



- Synthesis & Characterization
- Experimental Data Collection

- Multi-Scale Modeling
- Technoeconomic Analysis

- Industry Adoption & Partnerships

Helping DOE build multi-scale, multi-disciplinary, multi-institutional programs to bridge the knowledge gaps for energy-centric post-combustion CO_2 separations for the global CCS community.

Industry Team Members

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NETL Project Manager: Sai Gollakota

Project Manager: David Heldebrant

RTI INTERNATIONAL

Marty Lail

- ***Bench-scale testing***
- ***Durability testing***
- ***Slip-stream prep***

EPRI ELECTRIC POWER RESEARCH INSTITUTE

Abhoyjit Bhown

- ***Data validation***
- ***Data needs***
- ***Process design***
- ***Power industry engagement***
- ***Slip-stream prep***

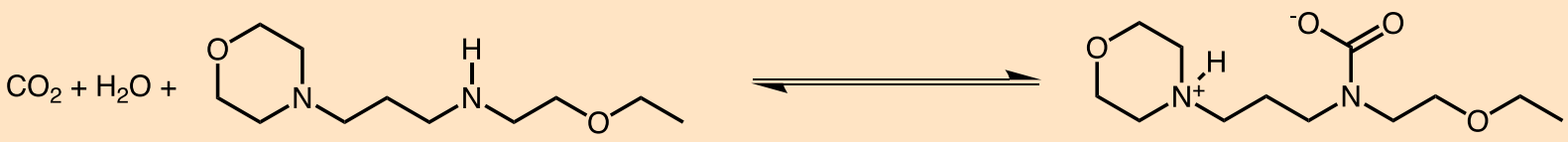
FLUOR®

Paul M. Mathias

- ***Modeling***
- ***Data validation***
- ***Data needs***
- ***TEA***
- ***Commercialization prep***

3rd Generation CO_2-Binding Organic Liquids (CO_2BOLs) – *EEMPA*

- Retains "water-lean" functionality (only 5-10% water in circulated solvent)
- Is a single-constituent solvent (not a blend)
- Exhibits shift in polarity upon loading with CO_2 (i.e. can leverage polarity swing)
- Overcomes past viscosity challenges (<50cp when fully loaded)
- Can operate in commercial absorber/stripper equipment
- Can be made at an economical price ($10/kg is current target)



EEMPA
N-(2-ethoxyethyl)-3-morpholinopropan-1-amine

Nature, (2005), 436, 1102; Ind. & Eng. Chem. Res. (2008); 47, 3, 539, Energy Environ. Sci., (2008), 1, 487;
RSC Adv., (2012), 3, 566-572; *Energy Environ. Sci (2013)*, 6, 2233 – 2242; *Energy Fuels*, (*2016*), *30*, 1192–1203;

Project Schedule

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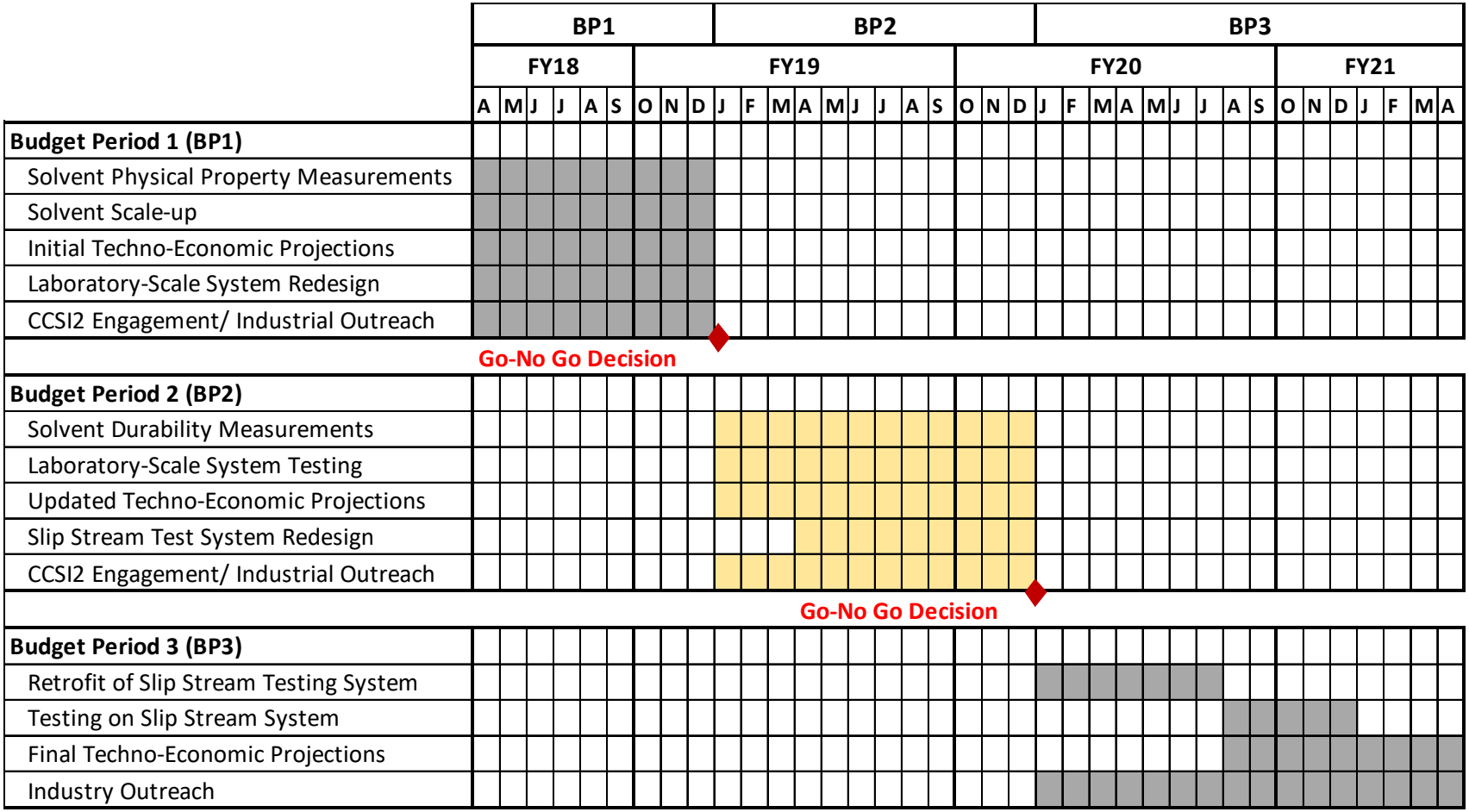

Budget Period 2 Milestones

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Project currently on track to meet upcoming Milestones.

Chemical degradation mechanisms quantified, necessary mitigation strategies developed for solvent. Solvent lifetime and makeup rates quantified.	9/29/2019
Independent durability testing complete for 1-4 derivatives. Chemical degradation mechanisms quantified, necessary mitigation strategies developed. Solvent lifetime and makeup rates quantified, most durable solvent identified for future testing.	9/29/2019
Continuous Flow Testing on 1 viable derivative completed. At least 40 hours of steady state 90% capture from simulated flue gas (15% CO_2, 85 % N_2 with SO_x, NO_x, O_2) with and without PSAR.	9/29/2019
Final TEA completed with costs targets at or below \$30/tonne CO_2	12/31/2019

Round-Robin Tests – EEMPA Solvent Thermodynamic Data with Model Predictions

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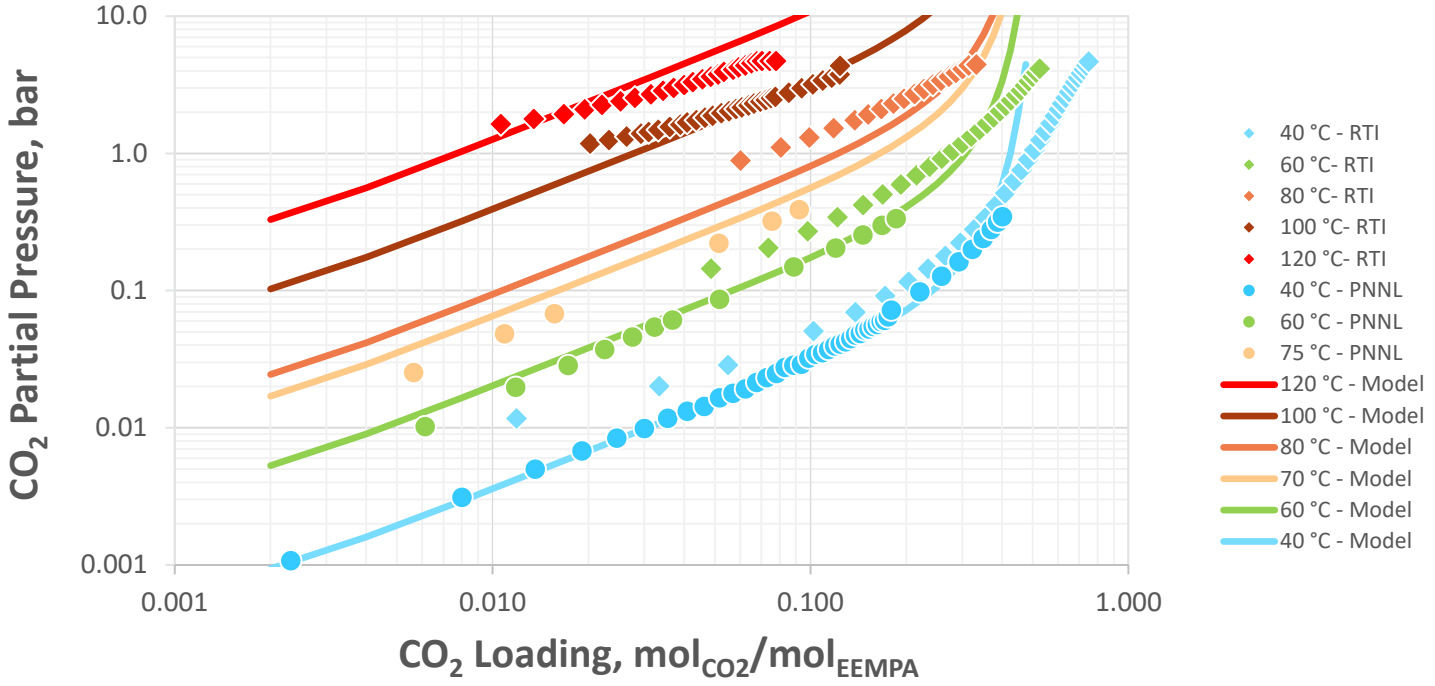
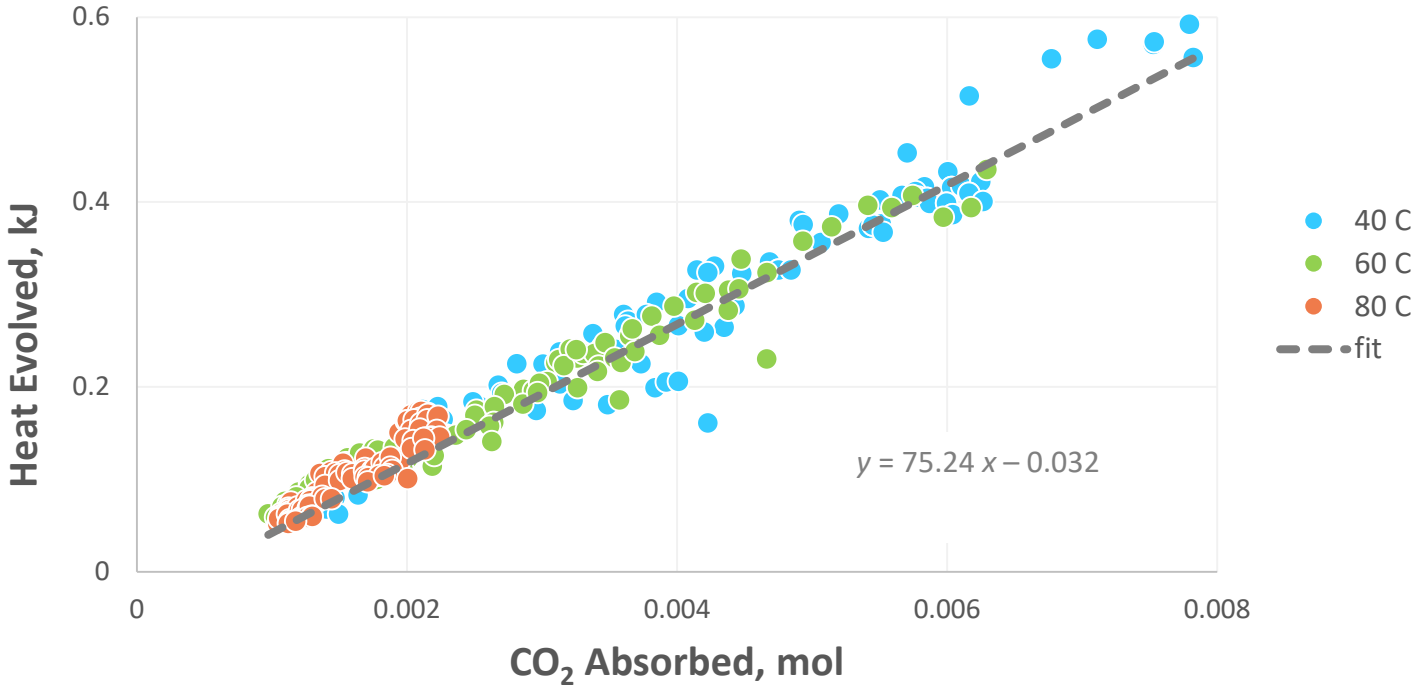
- Inter-laboratory thermodynamic data collection: PNNL and RTI.
- Independent data critique and rigorous analysis by project team: PNNL, RTI, EPRI, and Fluor Corp.
- VLE measurements from PNNL and RTI aligned well.
- Current model deemed adequately describes data in range of interest for capture process but further refinement possible with ongoing water-loaded data collection.



Round-Robin Tests - Solvent Thermodynamic Data with model predictions

- RTI measurements expanded to calorimetry and liquid density.
- Thermodynamic consistency established between calorimetry and VLE data according to Gibbs-Helmholtz relation.
- Independent EPRI analysis – Calorimetry data was filtered and weighted based on uncertainties estimated via Monte Carlo sampling.
- Calorimetry data indicates ΔH_{abs} = 75.2 ± 2.2 kJ/mol-CO_2 at 95% confidence.



Initial Techno-Economic Projections
Preliminary Process Model

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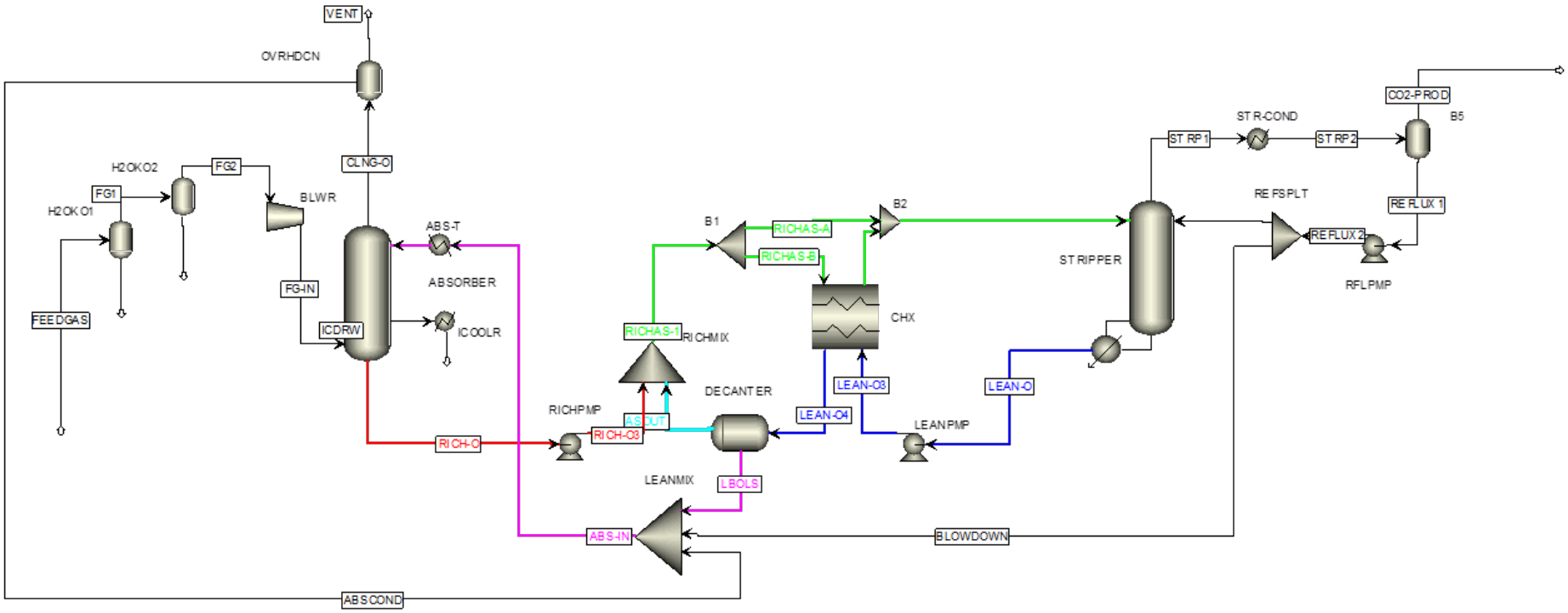

- Process configured similar to NETL Case 10 with 90% CO_2 capture.
- PSAR not yet incorporated; be added if needed.

Initial Techno-Economic Projections
Summary of Results

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	MEA (NETL Case 10)	EEMPA w/o PSAR	EEMPA + PSAR (Expected Impacts)
Lean Loading, $mol_{CO2}/mol_{solvent}$	0.27	0.05	
Rich Loading, $mol_{CO2}/mol_{solvent}$	0.49	0.23	
Water content, wt%	69.3	2.8	
Regeneration Temperature, °C	118	117	↘
Reboiler Duty, $GJ/tonne_{CO2}$	**3.66**	**2.17**	≈
Equivalent Work, kJ_e/mol_{CO2}	**52.4**	**33.2**	↘
Net Plant Efficiency,	**25.4**	**29.1**	↗
CAPEX of CDR, MM$	**443**	**464**	↗
Mitigation Cost, $/$tonne_{CO2}$	**66.5**	**52.2**	

- EEMPA has lower OPEX Case 10 and comparable CAPEX.
- Potentially additional cost reduction with PSAR.

Solvent Durability – Oxidative and Thermal Degradation

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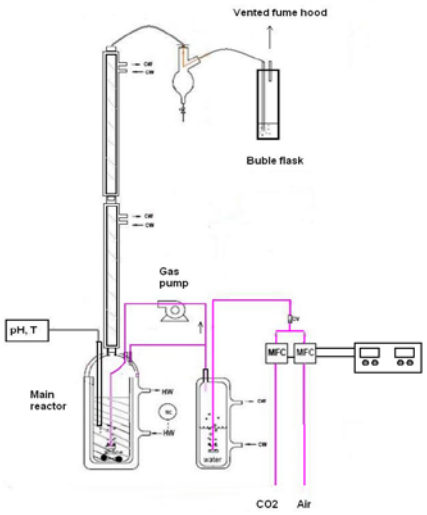
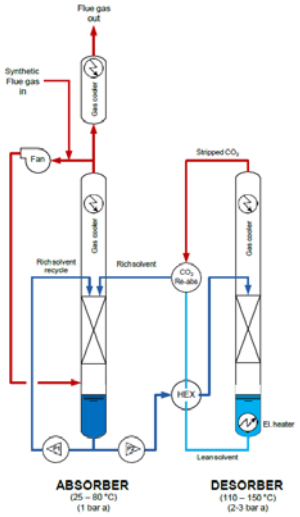
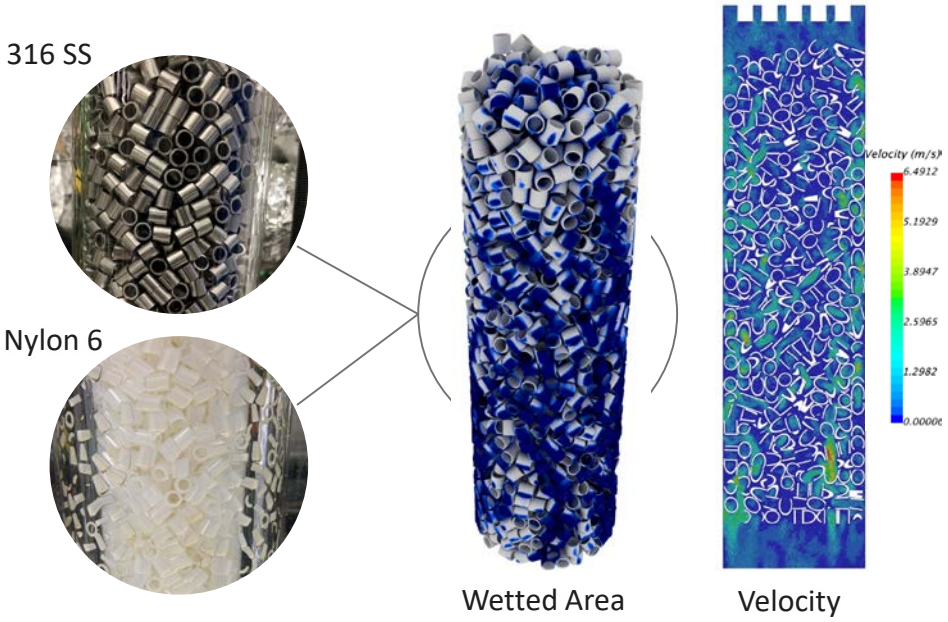
- RTI/SINFEFF-lead durability tests are ongoing.
- Thermal degradation – 117°C for 5 weeks in N_2 with 300-series stainless steel, dry and water-loaded EEMPA
- Oxidative solvent degradation – tests under both absorber and stripper conditions and with oxygen, NOx, SOx planned.

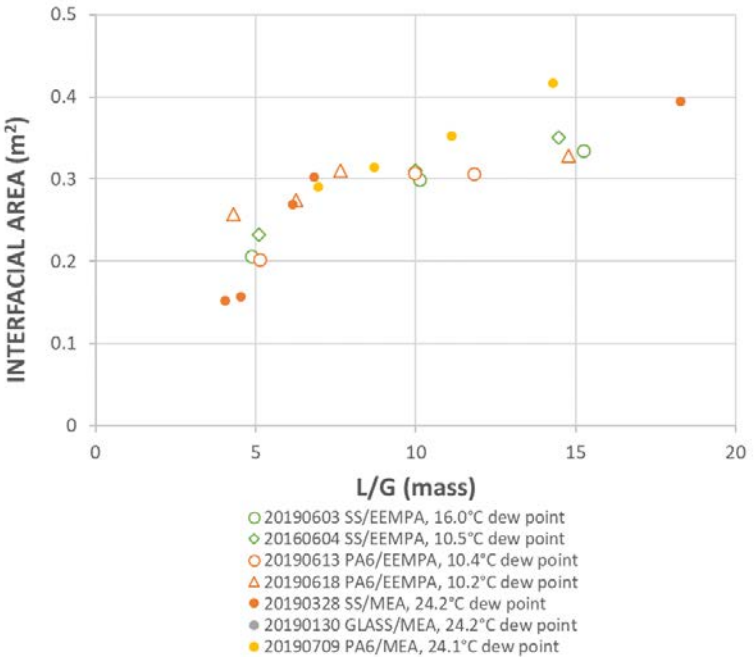




Collaboration with CCSI²

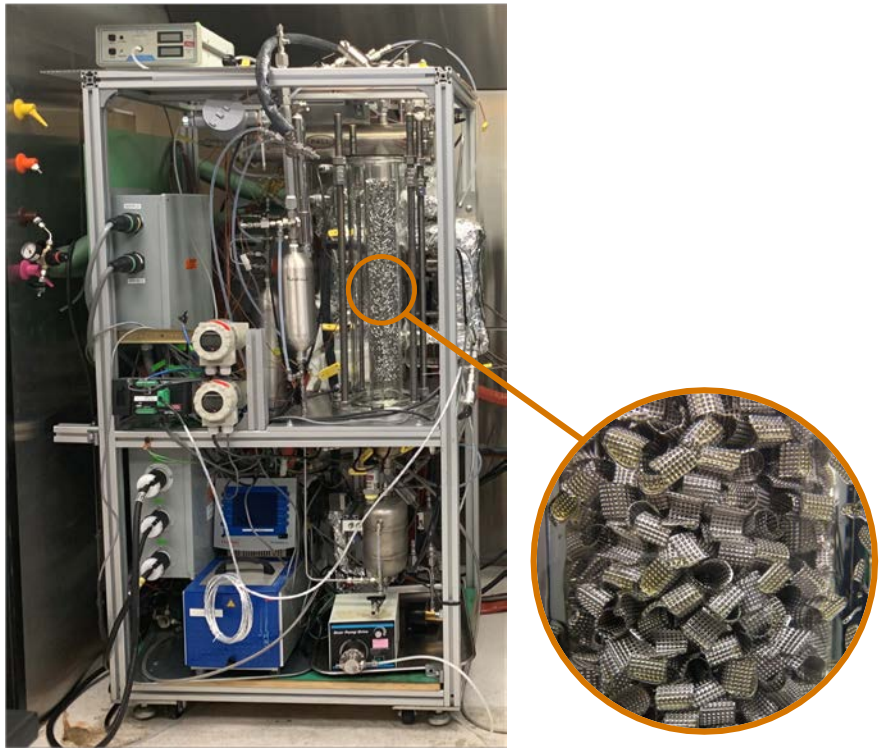
- CFD-based hydraulic model developed to predict effective interfacial area.
- Model validation using LCFS data with both MEA and water-lean solvents evaluated on both metal and plastic random packings.
- Further laboratory-scale solvent testing is aided by design of experiments with model guidance.

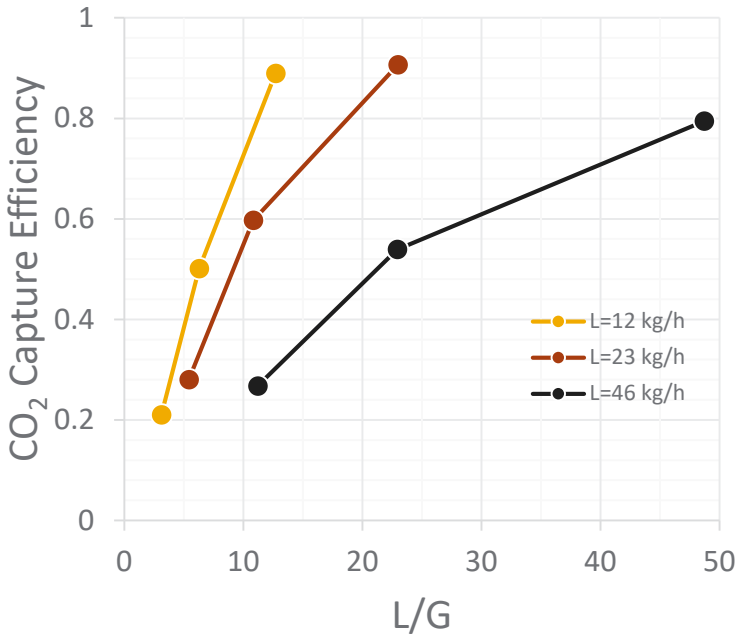




CCSI² Carbon Capture Simulation for Industry Impact

Laboratory Scale System Testing





- Ongoing parametric EEMPA CO_2 absorption tests leveraging CCSI^2 SDoE.
- Full flow loop long-duration tests are 40 hr+ onstream with NOx and SOx.

Summary

- Round-robin solvent property tests completed through strong collaboration with industry team. Data consistency increases confident level in current thermodynamic and process models.
- Initial TEA projected reboiler duty 40% lower than MEA. Total capture cost ~\$52.2/tCO_2 without process optimization. Additional PSAR data suggest the potential to reduce costs further, approaching the \$50/tCO_2 target.
- EEMPA oxidative degradation observed to be 42% lower than MEA. Ongoing extended durability tests by industry partners to confirm solvent lifetimes.
- CCSI^2 capabilities leveraged to improve model predictions and to guide lab-scale testing by design of experiment.

Acknowledgements

Pacific Northwest NATIONAL LABORATORY

Project Manager
David Heldebrant

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Capture Program: Lynn Brickett
NETL Project Manager: Sai Gollakota

Solvent Development

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Molecular Theory

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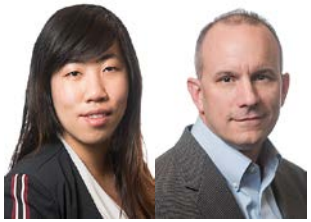
Testing and Analysis

Richard Zheng, Greg Whyatt, Andy Zwoster, Dushyant Barpaga

Process Modeling



Yuan Jiang, Charles Freeman

RTI INTERNATIONAL, EPRI, FLUOR®, CCSI² Carbon Capture Simulation for Industry Impact, Molecular Knowledge Systems — Designing Better Chemical Products

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