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

[Discovery of Carbon Capture Substances and Systems (DOCCSS)]
[NETL/DOE Project Manager: Sai Gollakota]

DAVID J. HELDEBRANT
PROJECT KICKOFF
MORGANTOWN, WV
SEPTEMBER 15, 2017

Overview of FWP-70924

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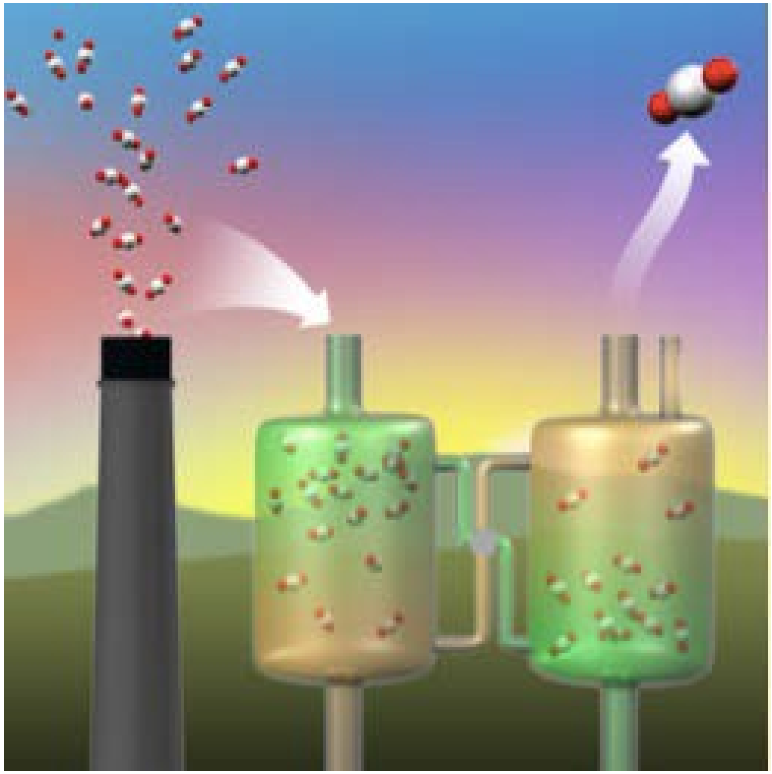
- Program Goals and Objectives
- CO_2BOL/PSAR Technology Background
- Program Overview
  - Overview of Tasks
  - Facilities and Capabilities
  - Program schedule BP1 & BP2
    - Task breakdowns
    - Success criteria
  - Project Budget
  - Risk Matrix
  - Project Deliverables
  - Future testing/commercialization
  - PNNL Team and Collaborations



PNNL FY16 at a glance

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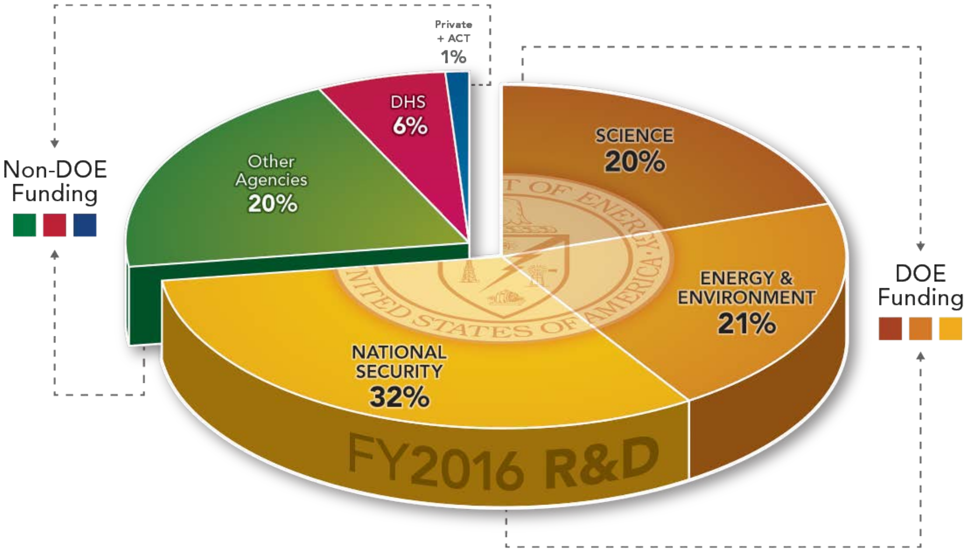
- $920.4M in R&D expenditures
- 4,400 scientists, engineers and non-technical staff
- 104 U.S. & foreign patents granted
- 2 FLC Awards, 5 R&D 100
- 1,058 peer-reviewed publications



Project Goals and Objectives

Goals

- Comprehensive physical and thermodynamic property testing of 1-BEIPADIP-2-BOL
- Project the energetics (e.g. reboiler duty, parasitic load) and preliminary cost analysis using Aspen Plus Modelling
- Develop technology that meets DOE's cost and performance baselines for post-combustion CO_2 capture.
- Collaborations with industry, national lab and academia through the Carbon Capture Simulation for Industry Impact ($CCSI^2$) program.
- Transfer to industry

Objectives

- Scale-up low-viscosity CO_2BOL derivative (1-BEIPADIP-2-BOL).
- Perform testing and evaluation through laboratory scale to inform techno-economic assessment of solvent performance towards DOE's target capture cost of $30 per metric ton of CO_2.
- Identify data needs and collect necessary data to support future scale-up of the solvent manufacturing and capture processes.

CO_2-Binding Organic Liquids (CO_2BOLs)

"Water-lean" organic switchable ionic liquid solvent system.

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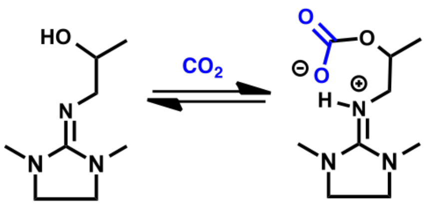
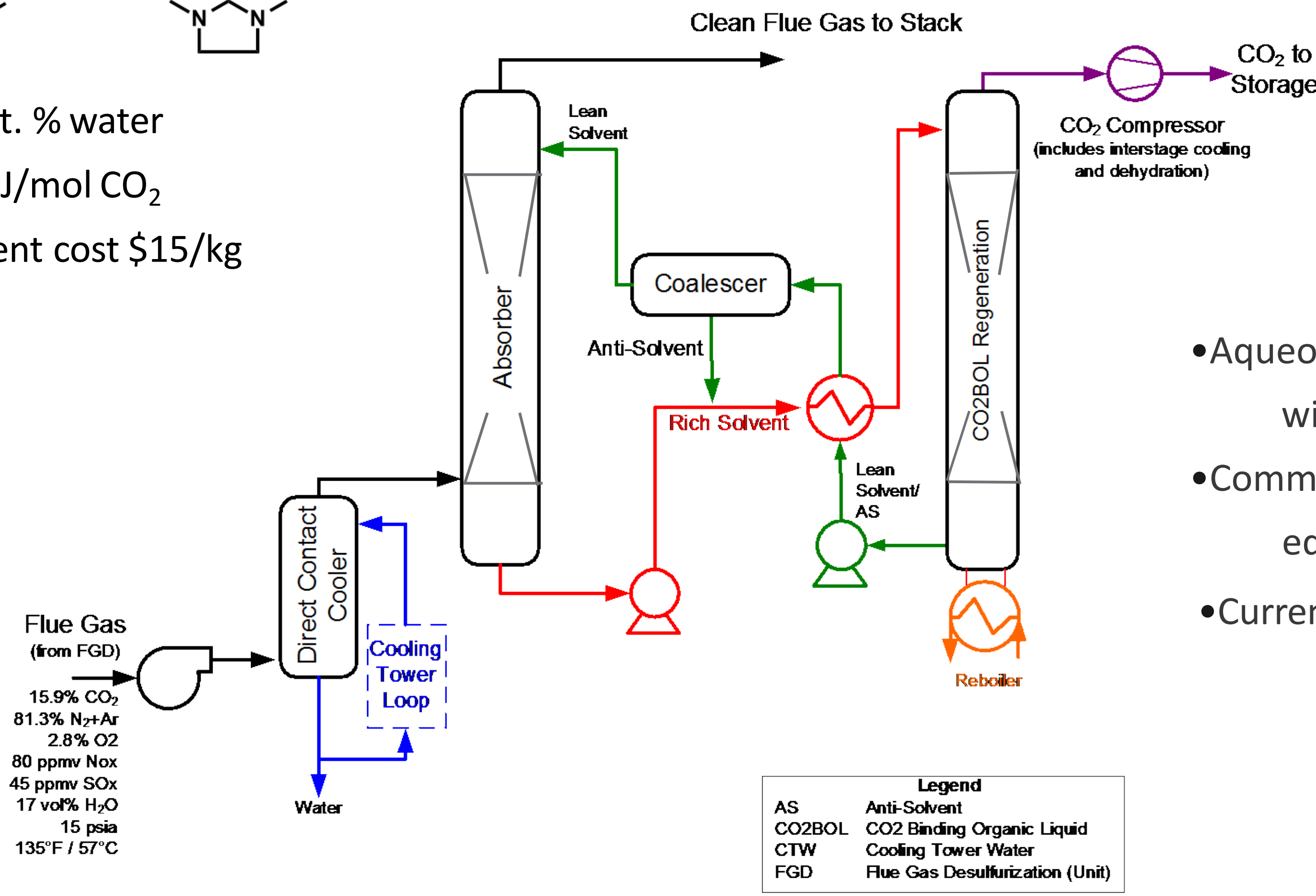


- ~5 wt. % water
- -80 kJ/mol CO_2
- Current cost $15/kg



- Aqueous amines design with added PSAR
- Commercially available equipment
- Currently un-optimized

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;

Polarity-Swing Assisted Regeneration (PSAR)

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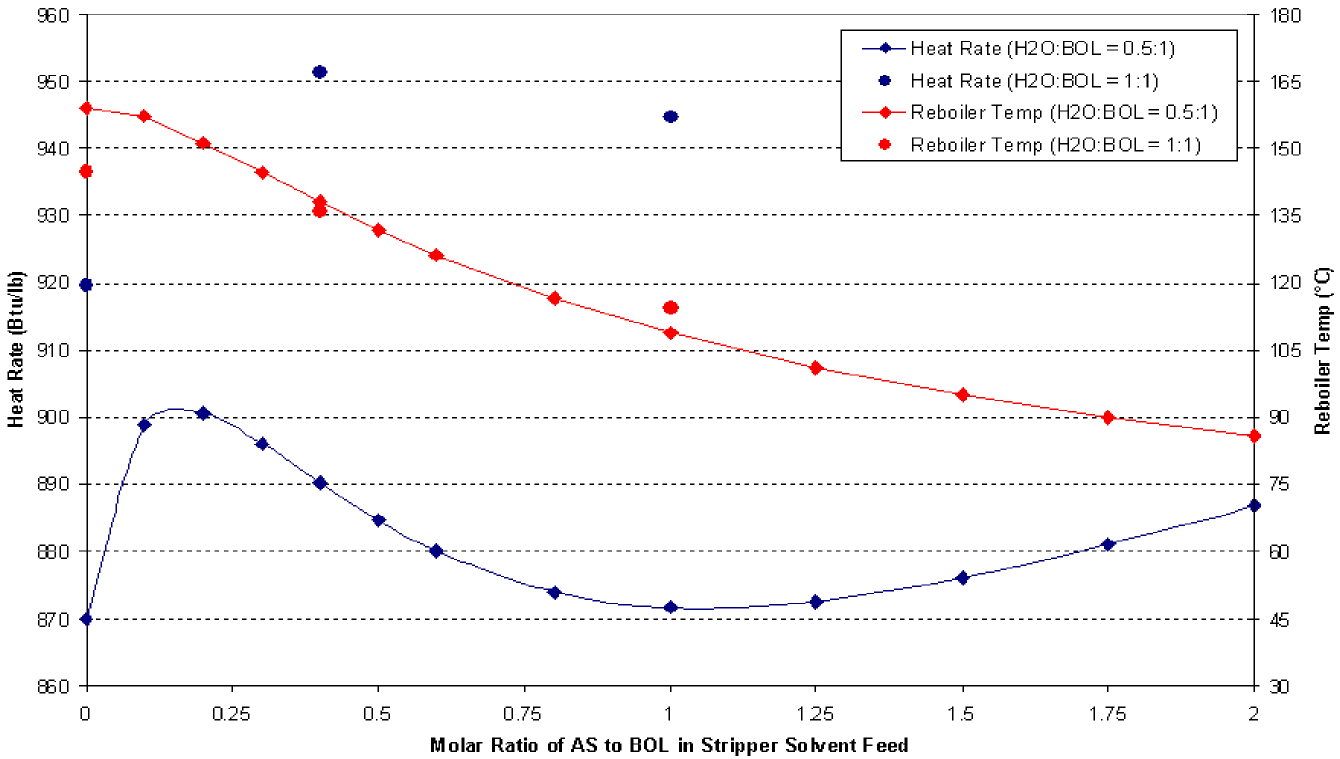
Maintains Reboiler Heat Duty but decreases T_{regen} by destabilizing the CO_2 carrier.

NETL baseline: 1520 btu/lb CO_2

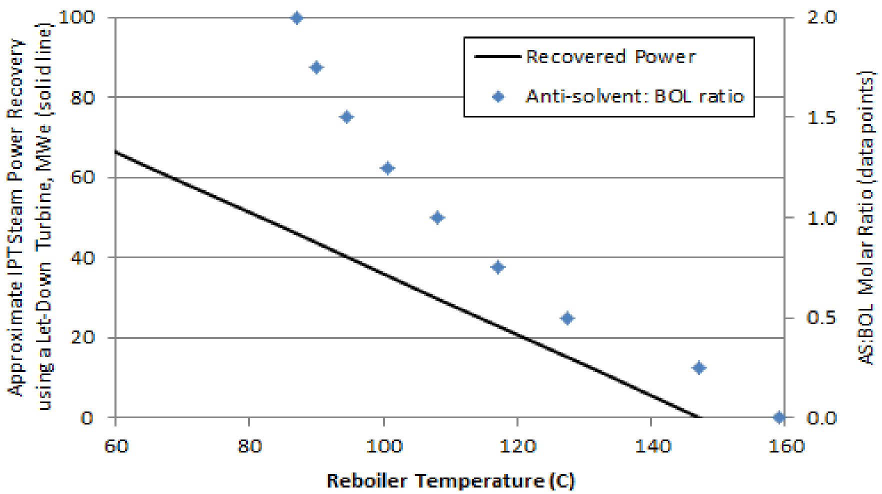


- Addition of hexadecane “antisolvent” equivalents
- 72 ˚C decrease in reboiler temperature
- Reboiler heat duty remains unchanged
- Sensitive to water

Energy Environ. Sci. ***(2013)*****,** 6, 2233 – 2242. U.S Patent NO: 9,707,508

Polarity-Swing Assisted Regeneration (PSAR)

May Increase Net Power Output by 102 Mwe (550 Mwe baseline).



- Extract power via a let-down turbine before passing the lower temperature steam to the reboiler
- Uses more steam than directly condensing IP steam from the plant power cycle but the power generated more than compensates.

Antisolvent Loading (Molar Equivalent)	Regeneration Temperature (°C)	Net Electric Power Produced (MWe)	Parasitic Load
0	159	594	25%
0.5	132	603	23%
1	109	621	21%
2	86	637	19%
TBD[1]	65	652	17%

[1]Based on projections of upper critical solution temperature

Energy Environ. Sci. (***2013***), 6, 2233 – 2242, U.S Patent NO: 9,707,508.
Assumes 20 cP *rich*-solvent

CO_2BOL/PSAR Catch-22

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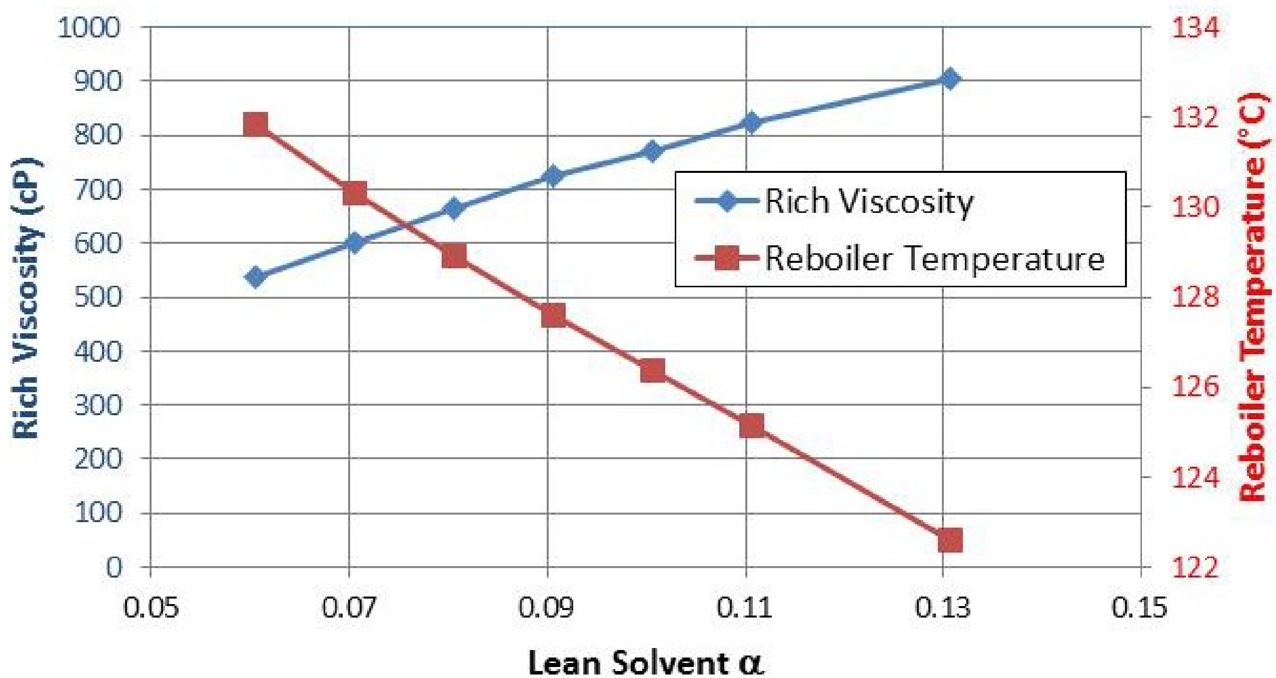
High rich-solvent viscosity negates the benefits of PSAR.



- Rich viscosity limits reboiler temperature and process performance
- Reduced viscosity allows higher α, which reduces $T_{reboiler}$ and reduces circulation rate
- Power plant efficiency benefit becomes significant when $T_{reboiler} < 100\ ^{\circ}C$

Energy Fuels, **2016**, *30* (2), pp 1192–1203

CO_2BOL Solvent Class…
Where we Left Off

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Process projected to be highly energy efficient but limited by viscosity.

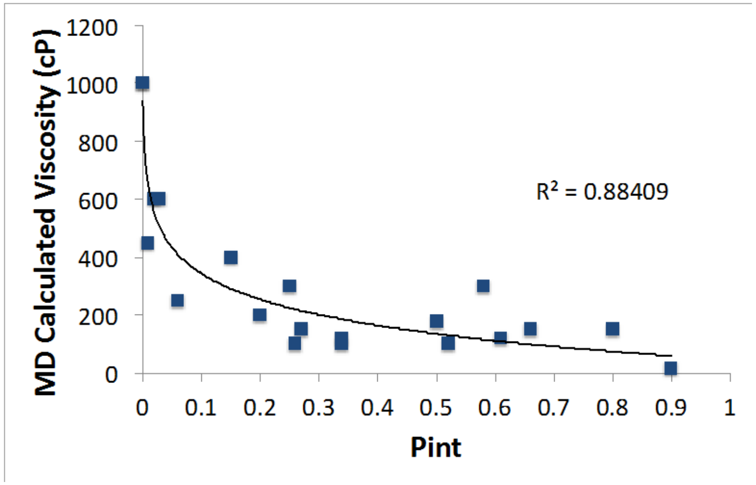
- 27% lower reboiler duty
- 2.1% higher net plant efficiency
- 2x's CAPEX
- Potential to meet DOE target

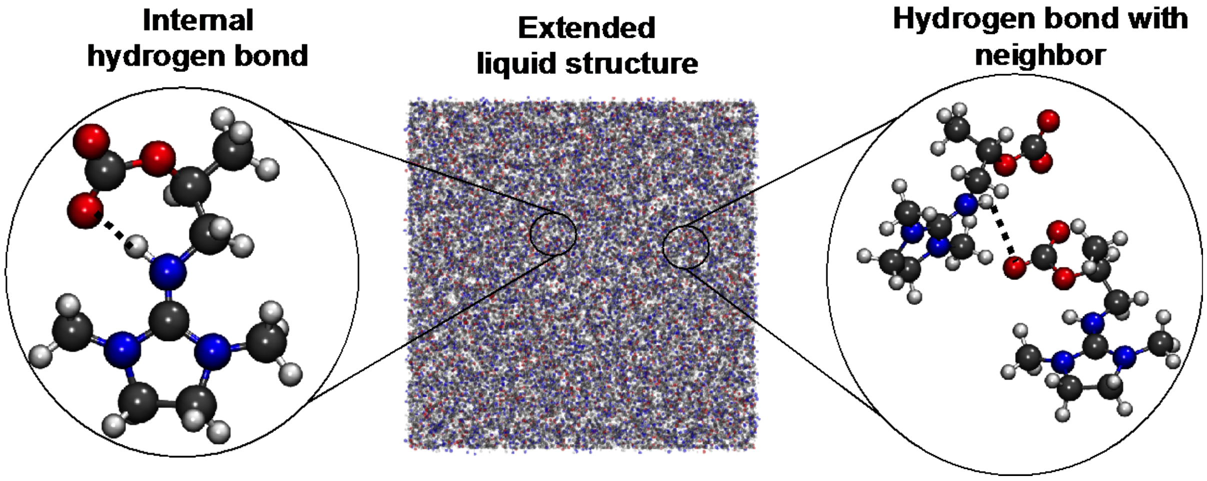
	NETL Case 10* – MEA capture	CO_2BOL/PSAR IPADM-2-BOL	CO_2BOL/PSAR IPADM-2-BOL 20 cP Theoretical**
Rich solvent viscosity (40 ˚C)	10	>353	20
Estimated Reboiler Duty (BTU/lb CO_2)	1520	1107	870
Net Plant Efficiency (HHV)	25.4%	27.5%	29.5%
Cost of CO_2 captured ($/tonne)	60	63	39

Energy Fuels, **2016**, *30* (2), pp 1192–1203

Viscosity Depends on Hydrogen Bonds Orientation

% of internal H-bonding (P_{int}) is the biggest descriptor of viscosity.



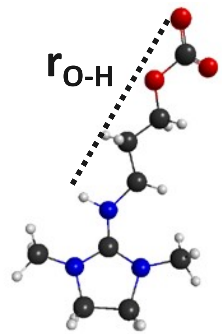


J. Phys. Chem. Lett., 2016, 7, pp 1646–1652

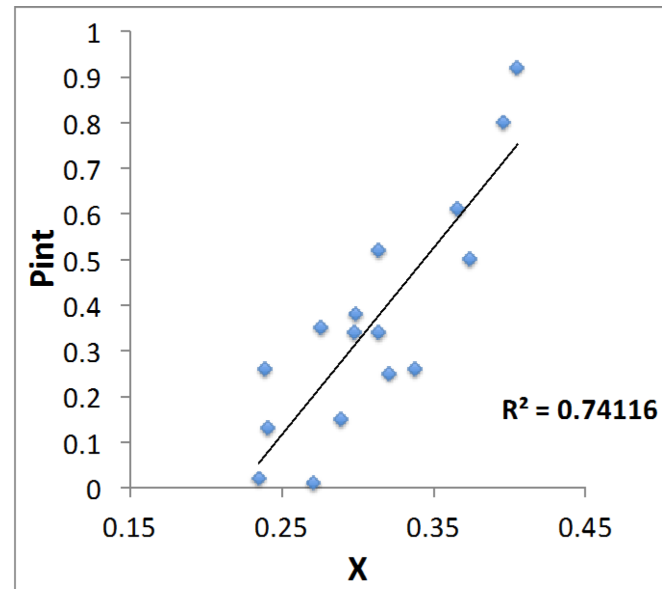
P_{int} From an Optimized Structure

Viscosity can be predicted without time intensive synthesis or modeling.

- If $\mathbf{r_{O\text{-}H}} > 2.0$ Å, then $\mathbf{P_{int}} = 0.001$

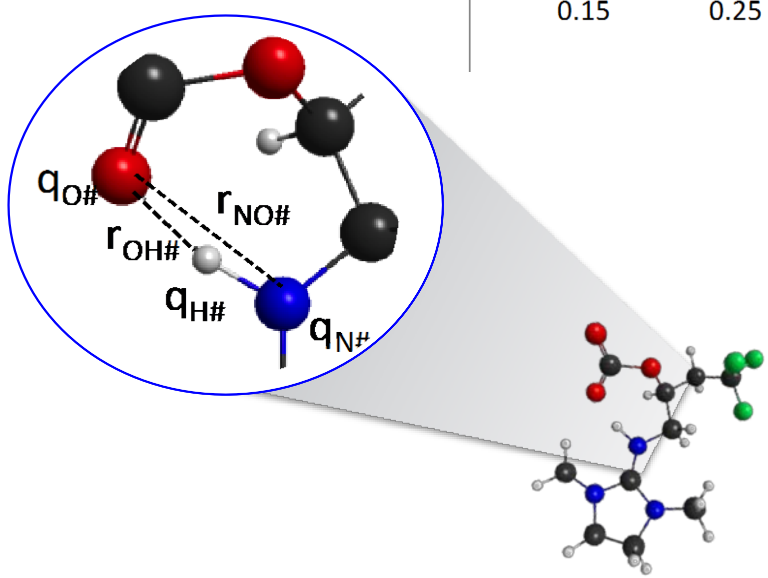


- If $\mathbf{r_{O\text{-}H}} < 2.0$ Å, then
- Difference between electrostatic repulsion (NO) and attraction (OH)



$$P_{int} = c_1 X + c_2$$

$$X = \frac{q_N q_O}{r_{NO}} - \frac{q_O q_H}{r_{OH}}$$



J. Phys. Chem. Lett., 2016, 7, pp 1646–1652

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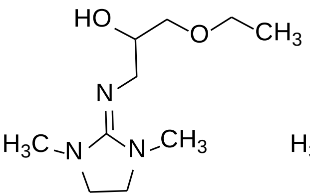
Designing 3rd Generation CO_2BOLs

500 Candidate molecules down-selected by the reduced model.



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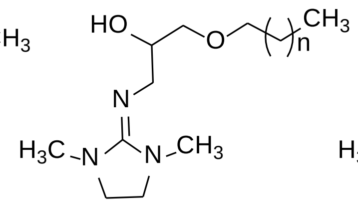
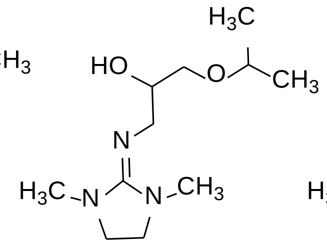


n = 1, 2

94,139



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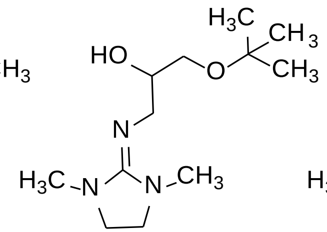

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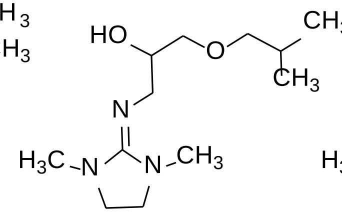

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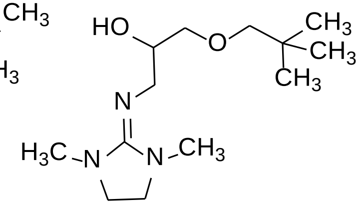

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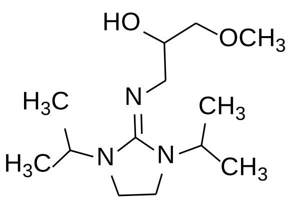

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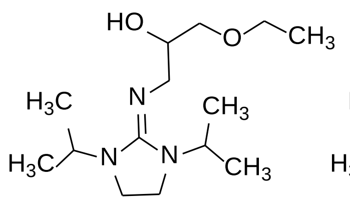

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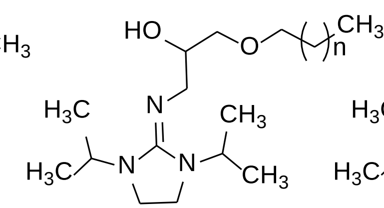
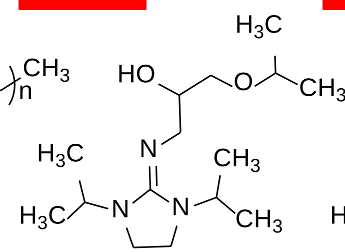


n = 1, 2

n/a, 14



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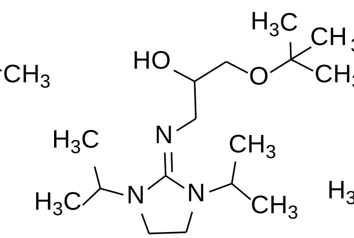

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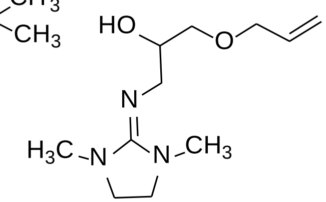
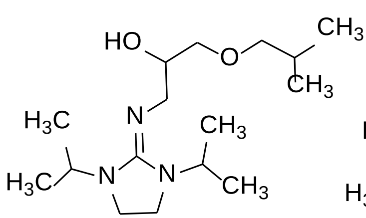


n/a



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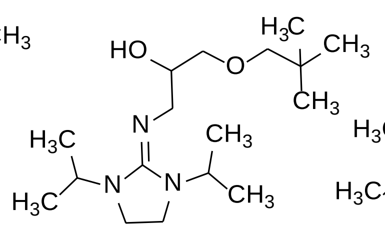
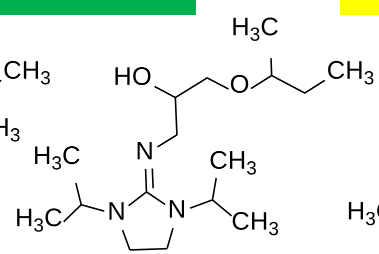


n/a



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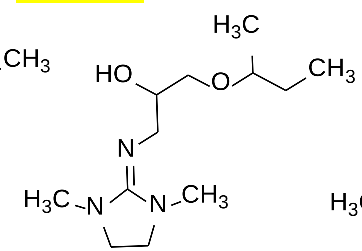

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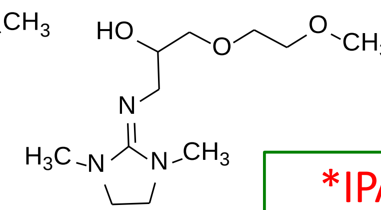

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*IPADM-2-BOL = 150 cP

High P_{int} Favors Neutral Alkylcarbonic Acid

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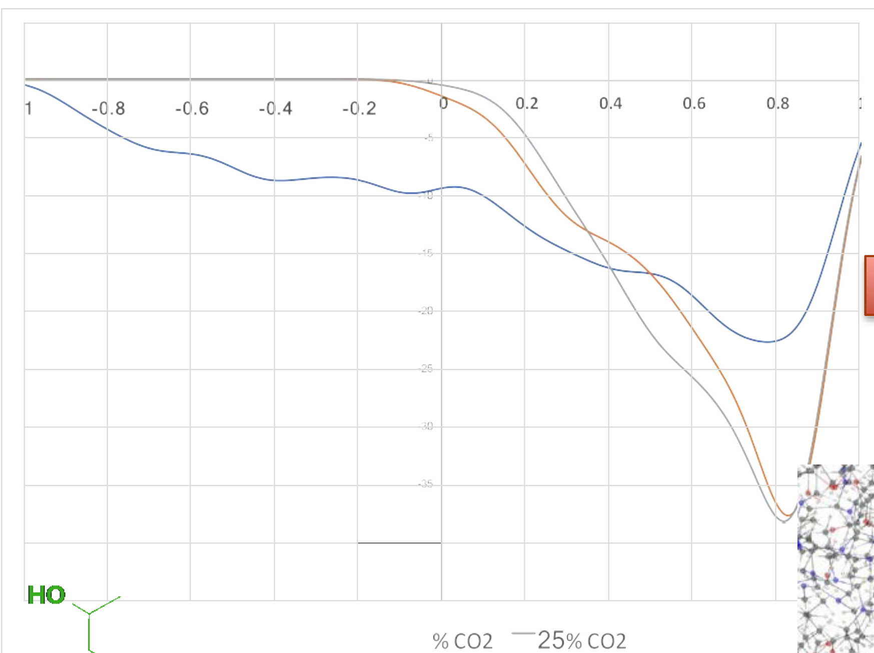
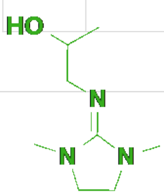
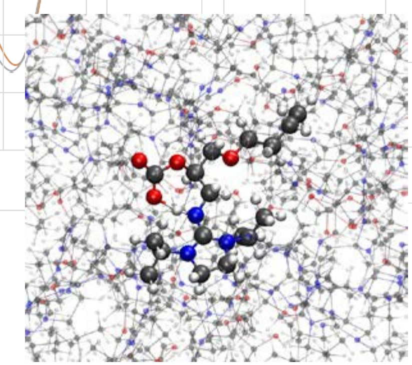
Internal H-bonding begins to favor "neutral" forms of capture, reducing the concentration of ions in solution.

ACID **ZWITTERION**

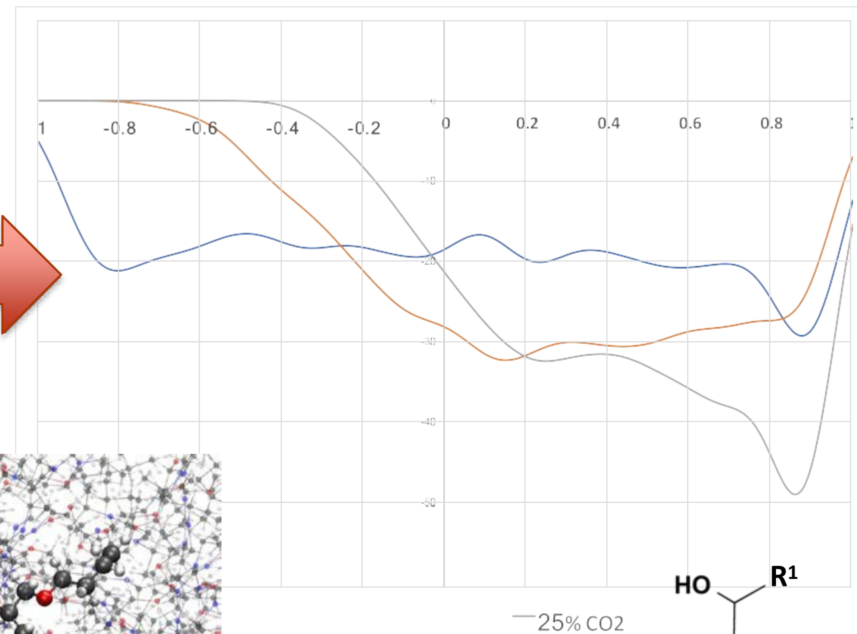




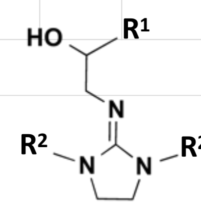
Initial



ACID **ZWITTERION**



After 10 ps



Malhotra *et al.*, *Manuscript In Preparation.*

Predicted Solvent Structure of Final Derivatives

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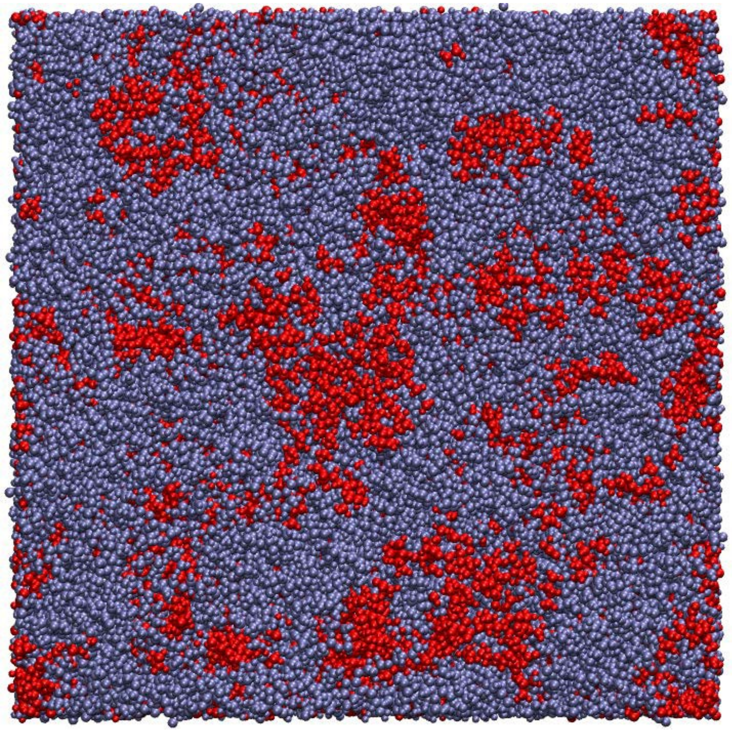
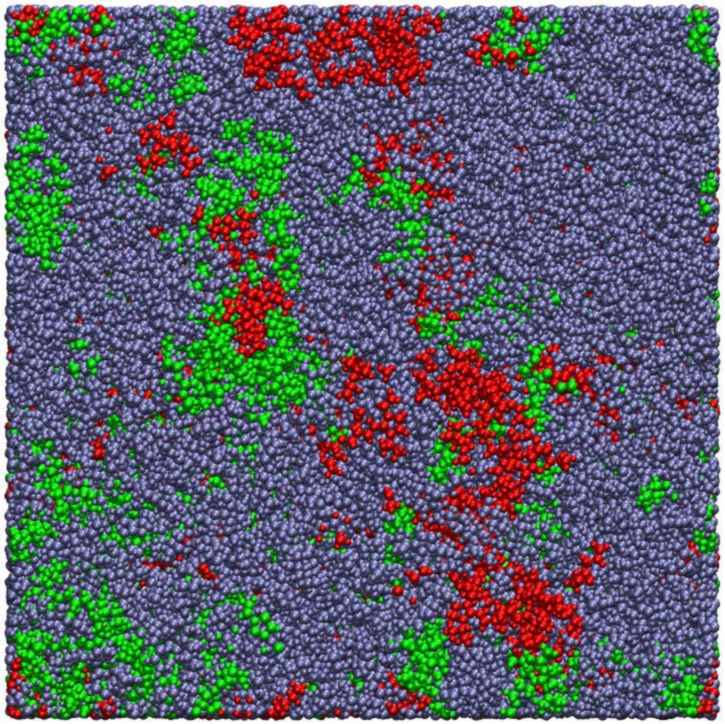
Solvents retain heterogeneous structure with reduced ionicity, still allowing for PSAR.



25% CO2 loading, all Zwitterion



25% CO2 loading, 1:1 acid:Zwitterion

Malhotra *et al.*, *Manuscript In Preparation.*

High P_{int} and Neutral Capture Combined

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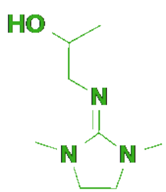
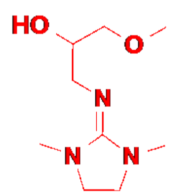
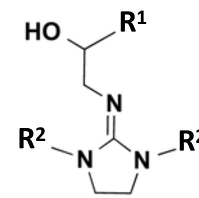
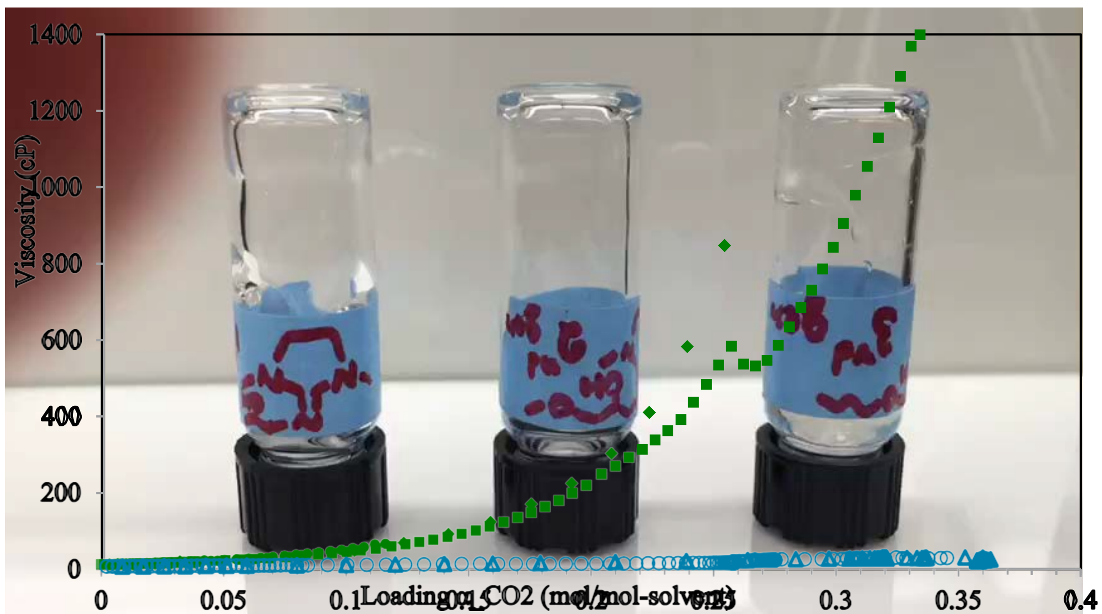
New derivatives are 98% lower in viscosity.







IPADM-2-BOL @ 40 mol% CO_2
MEIPADM-2-BOL @ 35 mol% CO_2
BEIPADIPA-2-BOL @ 42 mol% CO_2



CO_2BOL Generations

Malhotra *et al., Manuscript In Preparation.*

3rd Generation Derivative Properties

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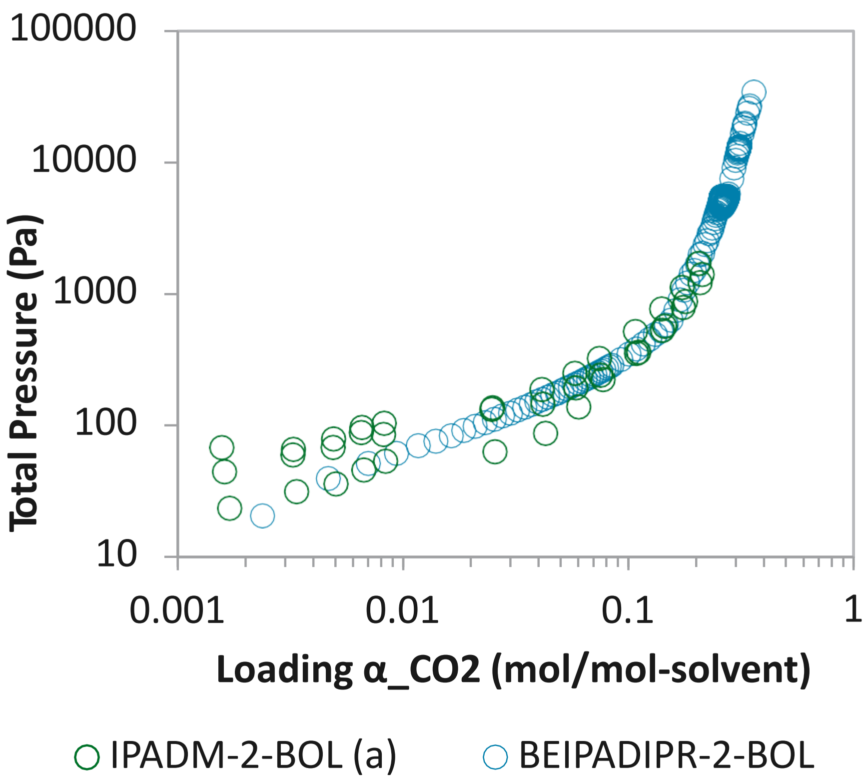
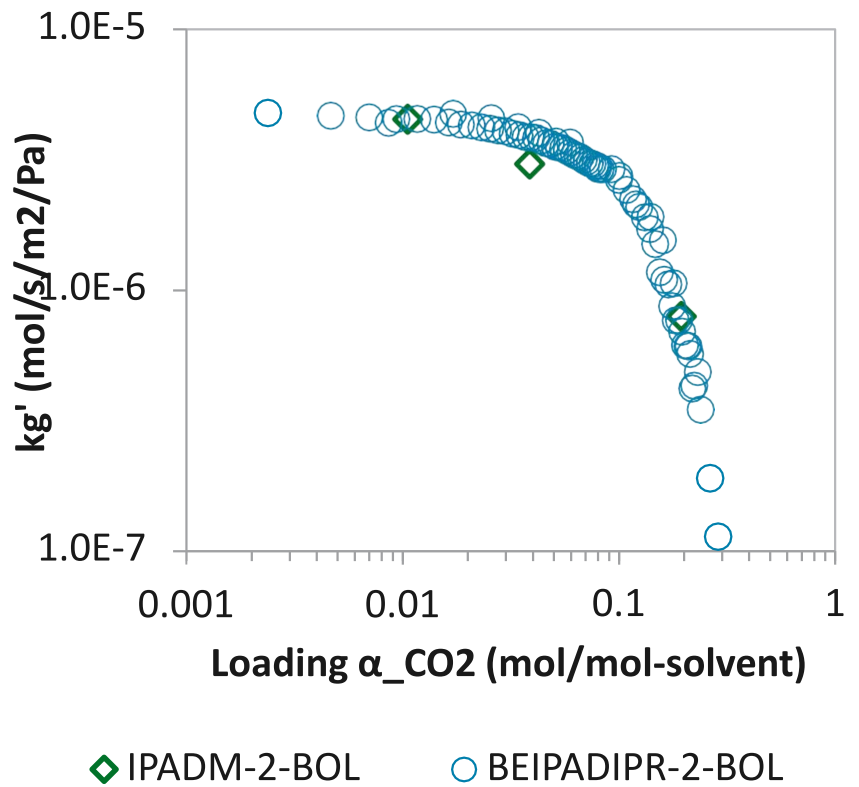
PVT testing shows physical and thermodynamic properties are retained.





- Comparable P* at 40 ˚C to IPADM-2-BOL at 40 ˚C
- Identical mass transfer of CO_2 (*kg'*) to IPADM-2-BOL at 40 ˚C

Malhotra *et al.*, *Manuscript In Preparation.*

CO_2BOL Solvent Class… Where We Are Now.

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Revised formulation is projected to be close in performance to theoretical case.

Potential:

- 40% lower reboiler duty
- 4% higher net plant efficiency
- Meet DOE's $40/tonne metric

	NETL Case 10* – MEA capture	CO_2BOL/PSAR IPADM-2-BOL	CO_2BOL/PSAR IPADM-2-BOL 20 cP Theoretical**	CO_2BOL/PSAR BEIPADIP-2-BOL
Rich solvent viscosity (40 ˚C)	10	>353	20	36
Estimated Reboiler Duty (BTU/lb CO_2)	1520	1107	870	TBD
Net Plant Efficiency (HHV)	25.4%	27.5%	29.5%	TBD
Cost of CO_2 captured ($/tonne)	60	63	39	TBD

Whyatt *et al., Manuscript In Preparation.*

CO_2BOL Solvent Class…
Where We Are Now.

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CO_2BOLs/PSAR have a higher percentage of theoretical minimum work than aqueous amines.

$$W_{eq} = W_{heat} + W_{pump} + W_{comp}$$ *

$$W_{heat} = \eta_{stm-tb}\left(\frac{T_{stm,sat} - T_{sink}}{T_{stm,sat}}\right) Q_{reb}$$

$$W_{pump} = \frac{\dot{V}_{rich}(P_{strp} - 1\ bar)}{\eta_p}$$

$$W_{comp}\left(\frac{kJ}{mol\ CO_2}\right) = 15.3 - 4.6 lnP_{in} + 0.81(lnP_{in})^2 - 0.24(lnP_{in})^3 + 0.03(lnP_{in})^4$$

$$1\ bar \le P_{in} \le 149\ bar$$

2nd gen amines =~36 kJ/mol	Theoretical Minimum Work*	Recreated NETL Case 10 MEA capture[1]	CO_2BOL/PSAR IPADM-2-BOL 356 cP[1]	CO_2BOL/PSAR IPADM-2-BOL 20 cP Theoretical[1]**	CO_2BOL/PSAR BEIPADIP-2-BOL 36 cP
RAW (kJ/mol CO_2)	18.2	44.1			
% minimum	100%	41.3%			

1. *Energy Fuels,* (2016), 30, 1192–1203. *Energy Environ. Sci.,* (2013), 6, 2233. CO_2BOL cases include 13 MW refrigeration duty.
*Lin, Y. J., Doctoral dissertation, U. T. Austin, 2016. ** Theoretical minimum, not experimentally observed.

Project Major Tasks

7/17/2017 – 12/31/2019

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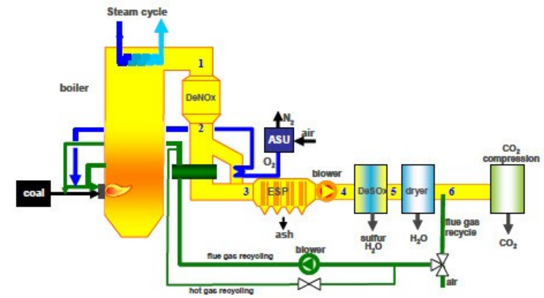
Solvent Scale-up

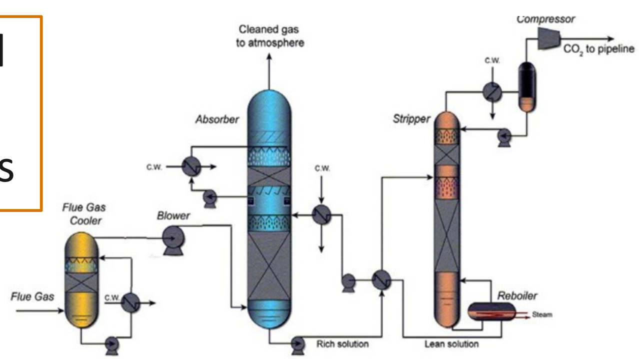
Parametric testing: O_2, SO_x, NO_x, H_2O



Kinetic Testing

Techno-economic Assessment

Absorber and Stripper Configurations



Industry Handoff

PNNL Facilities and Capabilities

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- Modeling work will be performed in the Math building using in-house clusters, and supercomputer facilities including EMSL (PNNL) and NERSC (LBNL)
- Synthesis and characterization: Physical Sciences Laboratory (PSL)
  - Nuclear Magnetic Resonance (NMR), Infrared Spectroscopy (IR), Calorimetry, 5-L synthesis reactor

- Kinetic and thermodynamic characterization will be performed in PNNL's Carbon Capture Laboratory ($2,200,000 in internal investments)
  - Facilities include wetted-wall column, PPVT cell & Mobile Bench-Cart, viscometers


5-L Synthesis Reactor


Continuous Flow Portable Cart


Wetted Wall

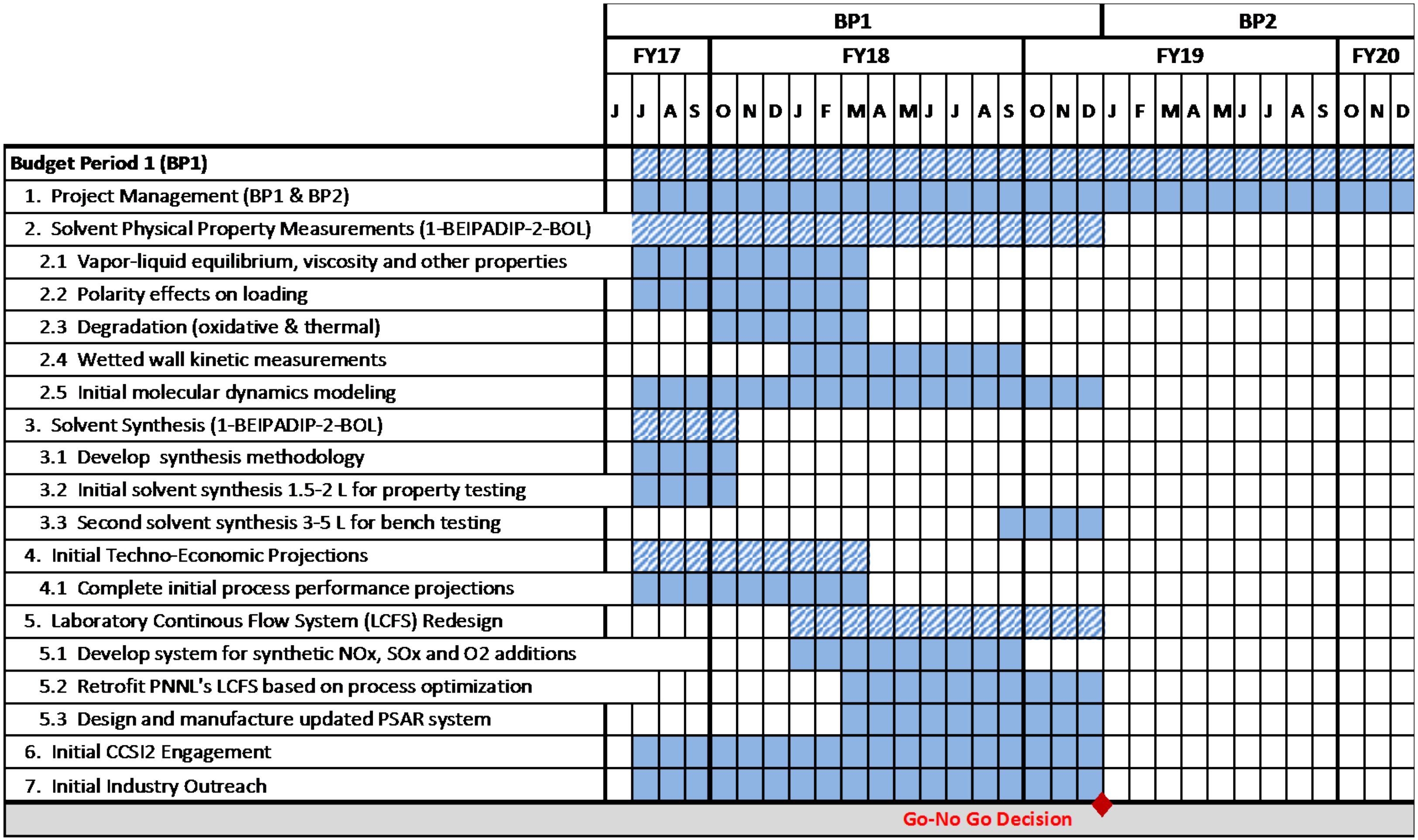
Technical Work --- Budget Period 1

- BP-1: Synthesis, characterization, property testing and continuous flow cart retrofit

- Work scope:
  - Synthesize 3 to 10 liters of 1-BEIPADIP-2-BOL for comprehensive property testing.
    - Three backup derivatives (i.e. 1-*s*-BEIPADIP-2-BOL, 1-*i*-BEIPADIP-2-BOL, 1-*n*-PEIPADIP-2-BOL) if there are any critical limitations (e.g. degradation, cost).
  - Measure physical and thermodynamic properties that are needed to project process performance.
  - Revise thermodynamic and kinetic models to revise ASPEN Plus models for projections of material performance, e.g. reboiler duty and equipment sizing.
  - Retrofit/redesign/shakedown laboratory test system to provide required information.
  - Preliminary techno-economic analysis (TEA)

Project Schedule by Task-BP1

7/17/2017 – 12/31/2018



Task 2: Solvent Physical Property Measurements (1-BEIPADIP-2-BOL)

- Physical and thermodynamic properties
  - Measure viscosity, density, VLE, vapor pressure, thermal conductance, contact angle and CO_2 uptake capacity of 1-BEIPADIP-2-BOL as a function of CO_2 and water loading
  - Vapor-Liquid Equilibrium curves will be measured with 2.5 5 and 10 wt% at 40 ˚C (projected absorber temperatures) in addition to 60 and 80 ˚C to extract heat of solution.

- Polarity effects on loading
  - Measure LLE phase diagrams for varied antisolvents with 1-BEIPADIP-2-BOL to determine miscibility temperatures and optimal antisolvent loadings
  - Asses antisolvent impacts on CO_2 release using PNNL's custom automated burette system
  - VLE measurements s at varied molar loadings of antisolvent to determine the polarity swing effects on equilibrium loading and kinetics.
  - The team will also investigate the viability of solid antisolvents to induce a PSAR.
  - Collaboration with LLNL to test 3-D printed packings to test the impacts (if any) of solid antisolvents and determine if the effect is linked to surface area of the packing.

Task 2: Solvent Physical Property Measurements (1-BEIPADIP-2-BOL)

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- Preliminary chemical durability studies
  - Quantify thermal degradation and hydrolysis rates at absorber and stripper conditions
  - *Operando* spectroscopy and post-mortem analysis using nuclear magnetic resonance (NMR), react infrared spectroscopy (IR), differential scanning calorimetry/thermal gravimetric analysis (DSC/TGA) and mass spectrometry (MS).

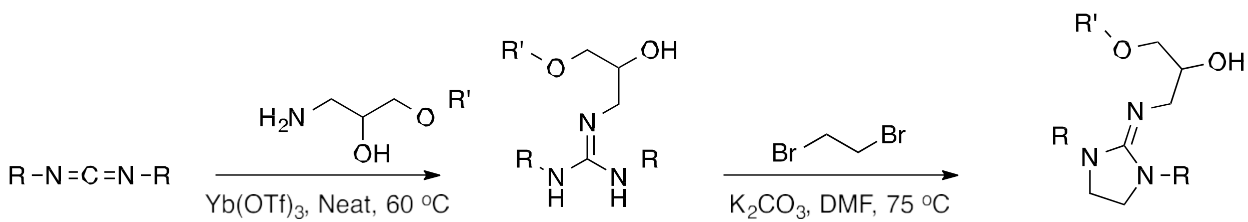
- Oxidative degradation studies will be performed in sealed pressure autoclaves under expected absorber and stripper conditions.
  - Testing all expected combinations of solvent, water, CO_2, and antisolvent
  - *Operando* spectroscopy and post-mortem analysis using NMR, IR, DSC/TGA and MS
  - If needed, assess chemical additives to retard the rate of oxidative degradation

- Kinetic measurements
  - wetted wall testing to measure the overall mass transfer coefficient K_G and gas and liquid-film mass transfer coefficients k_g and k'_g
  - Testing at 0, 5, 10 wt%) water loadings.

Task 3: Solvent Synthesis (1-BEIPADIP-2-BOL)

- Scale-up synthesis of 3-10L of 1-BEIPADIP-2-BOL
  - 1-2 L for wetted-wall testing
  - 100 mL for chemical durability testing
  - 3-5 L for continuous flow testing

- Develop synthesis methodology with costing projections ($10/kg)



Representative Scale-Up Synthetic Methodology

Task 4: Initial Techno-Economic Projections

Collaboration with Fluor and CCSI²:

- Revise thermodynamic and kinetic models (from FE-0007466)
- Assess alternative absorber and stripper configurations
- Assemble and optimize process flowsheet for 1-BEIPADIP-2-BOL
- Project reboiler heat duty, regeneration temperature, solvent circulation rate, and net power under thermal and PSAR regeneration methods.
- Qualitative equipment sizing in comparison to IPADM-2-BOL from (DE-FE0007466).
- Utilize NETL's Energy Data eXchange for input and tools to facilitate the TEA projections.
- Comparative cost analysis to assess viability towards reaching DOE’s $30/ton CO_2 target.

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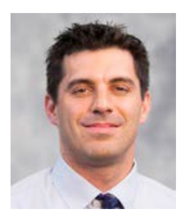
CCSI² Carbon Capture Simulation for Industry Impact

TEXAS The University of Texas at Austin

Dr. Paul M. Mathias



Michael Matuszewski

Professor Gary Rochelle

Task 5: Laboratory Continuous Flow System (LCFS) Redesign

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- Develop system for synthetic NOx, SOx and O_2 additions
  - Feed gas blending and system piping to deliver expected concentration ranges.
  - Multi-gas analyzer and sample gas conditioning systems
  - Liquid loops for handle liquid sampling and analysis
  - Sight glasses for visual detection of foaming and HSS formation
  - Reserve space and piping connections for solvent re-claimer loop if needed

- Retrofit based on process optimization and inputs from $CCSI^2$ and Fluor
  - Updated sizing for columns, exchangers, and pumps
  - Modular process configurations (stripper, absorber)
  - Configured for accurate mass and energy flow data

- Design and manufacture updated PSAR system
  - Novel contactor and fluid separator concepts
    - Advanced column packings additively manufactured

- Shake-down cart on 1^{st} generation (DBU:1-hexanol solvent)

Lawrence Livermore National Laboratory


Dr. Josh Stolaroff

Task 6: Initial $CCSI^2$ Engagement

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- Work in collaboration with the $CCSI^2$ team to develop detailed models of candidate capture technologies using multi-scale simulation tools.
- Provide input on data collection, initial techno-economic projections of the full-scale technology, and inputs to the laboratory-scale test system re-design.

Task 7: Initial Industry Outreach

- Industry outreach to assure that the technology attributes are clearly conveyed to a broad set of known developers.
- Fluor Corporation initial targeted industry due to their prior collaborations with PNNL and their expressed interest in advanced solvents that could hold commercial advantage.
- Industry outreach will occur through the $CCSI^2$ Industry Advisory Board.

Success Criteria- BP1

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Fiscal Year	Date	Success Criteria
2018	3/31/2018	Degradation mechanisms identified for 1-BEIPADIP-2-BOL with flue gas impurities and any necessary mitigation strategies developed to maintain solvent lifetime comparable to MEA
2018	9/29/2018	1-BEIPADIP-2-BOL exhibits k'g equal or greater than monoethanolamine (MEA) (7.64×10^{-6} mol s^{-1} m^2 Pa^{-1} at 40˚C) under a comparable driving force and a projected reboiler duty at least 30% lower than MEA (i.e. less than 1,064 btu/lb CO_2).

- 1-BEIPADIP-2-BOL exhibits *k'g* equal or greater MEA under a comparable driving force.
- Oxidative degradation mechanisms quantified and any necessary mitigation strategies developed.
- Projected reboiler duty at least 30% lower than MEA
- Two or more laboratory system redesign options evaluated for optimum performance and relevance to producing necessary data.
- Key equipment in redesign: absorber, stripper and polarity swing units.
- Revised laboratory test system configuration, with $CCSI^2$ and Fluor guidance, provide scale-up prediction accuracy within 80%.
- ***Go no-go presentation in December 2018**

Technical Work --- Budget Period 2

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- BP-2: Continuous flow and parametric testing.
- Work Scope:
  - Continuous flow parametric testing to assess absorber and stripper performance in addition to chemical durability.
  - Polarity-Swing Assisted Regeneration (PSAR) will be introduced to the system to confirm the magnitude of reboiler temperature decrease.
  - Testing will then proceed on simulated flue gas for 40 or more hours at steady state. Steady-state capture
  - Quantification of heat-stable salt formation with SOx, NOx, potential hydrolysis, and oxidative degradation.
  - Project solvent lifetime and subsequent make up rates.
  - Final TEA (partnership with Fluor Corporation and CCSI[2]).
  - Identify data needs and necessary data to support future scale-up of the solvent manufacturing and capture processes.
  - Assess potential to reach DOE's target capture cost of $30 per metric ton of CO_2.

Project Schedule by Task-BP2

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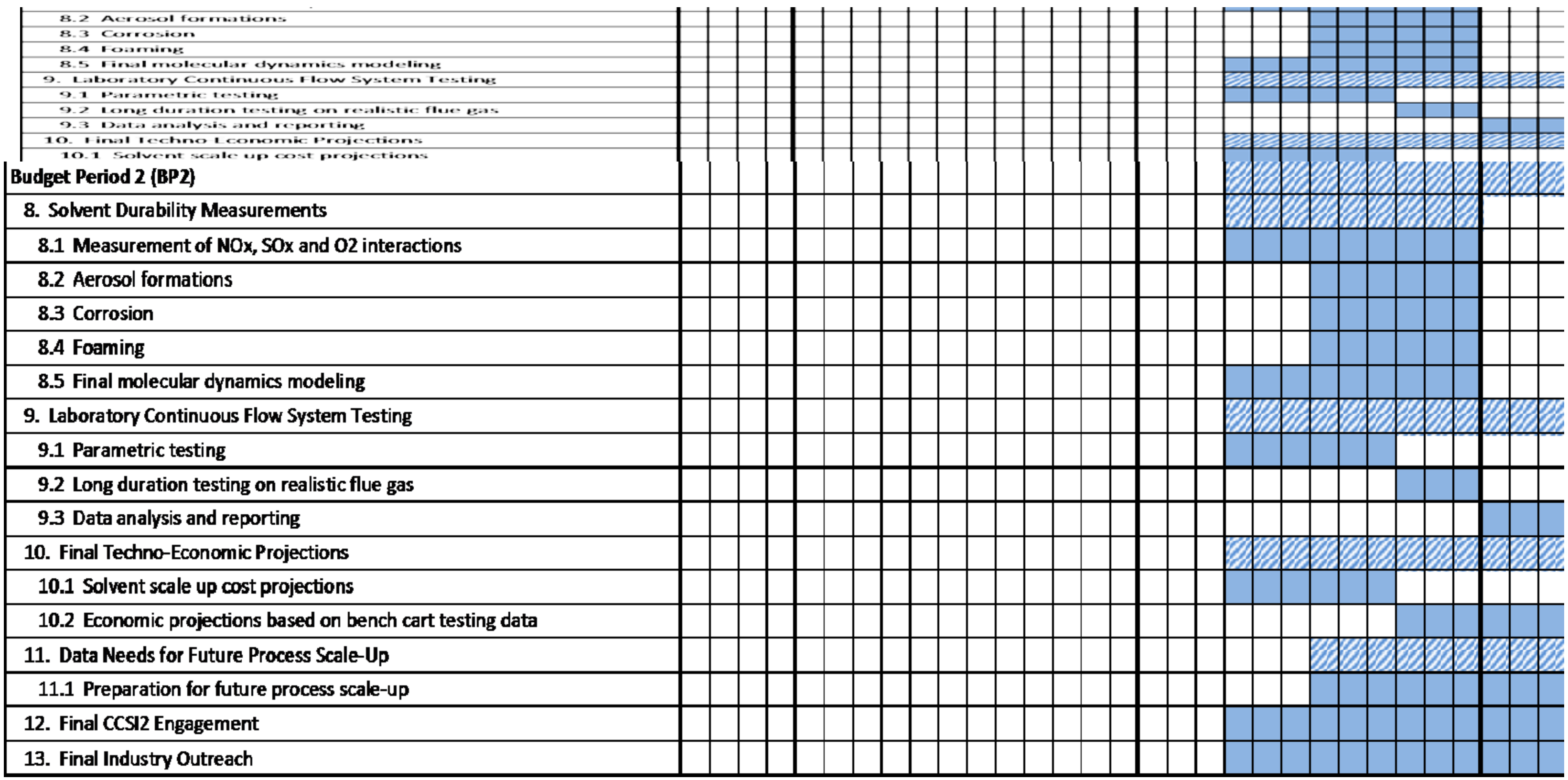
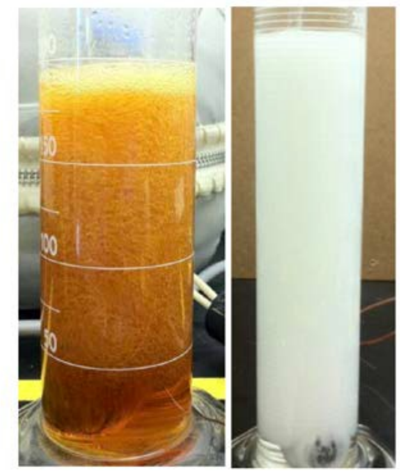
1/1/2019 – 12/31/2019



Task 8: Solvent Durability Measurements

- Parametric tests to identify and quantify degradations and make-up rates from SO_x, NO_x, HCl and O_2 using simulated or bottled flue gas.
- Reclaim HSS and assess methods to regenerate them
  - Thermal, PSAR, acid/base workup, ion exchange resins
- Investigate propensity to form nitrosamines
  - Quantify the formation rate and mitigation strategies
- Visual tests for aerosol formation, and (if needed) develop means to mitigate
- Visual tests for foaming using International Association for Testing Materials (ASTM) D1881-73 testing method
- Corrosion testing using installed coupons of carbon steel and 304, 304L, and 316L steels

COS CS_2 SO_2



Task 9: Laboratory Continuous flow system Testing

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- Baseline solvent testing: 3-5 liters of 1-BEIPADIP-2-BOL
  - Steady-state (40 hours) on simulated flue gas (15% CO_2 and 85% N_2) at 40 ˚C
  - Testing at varied water content (0-10 wt%) to determine optimal loading
  - Measure accurate mass and energy flow for the absorber and stripper
  - Assess column packings, structured, random, 3-D printed (LLNL)
- Addition of PSAR infrastructure
  - Novel contactor and fluid separator concepts
  - Steady-state (40 hours) on simulated flue gas (15% CO_2 and 85% N_2) at 40 ˚C
  - Assess optimal PSAR configuration and antisolvent circulation rates
- Parametric testing on realistic flue gas
  - Steady-state (40 hours) on bottled/simulated flue gas (15% CO_2 and 85% N_2) at 40 ˚C
  - Routine sampling of gas and liquid phases for: HSS of SO_x, NO_x, hydrolysis, and oxidative degradation
  - Visual inspection of foaming and aerosol formation
  - Corrosion testing on steel coupons

Task 10: Final Techno-Economic Projections

Collaboration with Fluor and CCSI²:

- Optimize final process flowsheet for 1-BEIPADIP-2-BOL
- Project reboiler heat duty, regeneration temperature, solvent circulation rate, and net power under thermal and PSAR regeneration methods.
- First-fill solvent costing with projected make-up rates
- Qualitative equipment sizing in comparison to IPADM-2-BOL from (DE-FE0007466).
- Utilize NETL's Energy Data eXchange for input and tools to facilitate the TEA projections.
- Comparative cost analysis to assess viability towards reaching DOE's \$30/ton CO_2 target.
- Recommendation to proceed for scale-up testing or industry handoff

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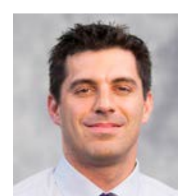
CCSI²
Carbon Capture Simulation for Industry Impact

Dr. Paul M. Mathias



Michael Matuszewski

Task 11: Data Needs for Future Process Scale-Up

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- Working with an established industry partner to prepare for next level of testing and subsequent hand off to industry.
- Projecting equipment configurations, size, cost and performance metrics for industry adoption or continued testing.
- Potential partners include:
  Fluor, RTI International, ExxonMobil, BASF

Task 12: Final CCSI² Engagement

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- CCSI² project team will be engaged to help with the re-assessment of the full-scale techno-economic projections based on laboratory-scale testing.
- Aid in design of the scale-up testing system design.
  - Control system design and sensor placement.
  - Infrastructure selection e.g. unit design and composition
  - Predict design and operational performance and develop a system that will produce the necessary data for the ultimate scaled-up system.

Task 13: Final Industry Outreach

- Companies will be specifically engaged to determine those who have interest in partnering on slip-stream demonstration system.
- Licensing discussions to make the associated business discussions compelling.
- Identify the industry partner prior to Tasks 11 and 12 enabling contribution to scale-up testing system design.

Success Criteria- BP2

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Fiscal Year	Date	Success Criteria
2019	9/29/2019	Continuous flow testing on derivative shows 90% capture from simulated flue gas (15% CO_2, 85 % N_2, SO_x, NO_x, O_2) for at least 40 hours with and without PSAR.
2020	12/31/2020	Final modeling projections using ASPENplus indicate an energy efficient process and potential (or a path forward) to achieve \$30/tonne CO_2 captured

- CO_2BOL/PSAR configuration capable of \$40/tonne CO_2 with potential for further optimization to meet \$30/tonne CO_2 target
- Synthetic costs can be met at \$10/kg
- Solvent lifetime and makeup rates quantified, with mitigation (if needed) strategies
- Industrial partner for further scale testing identified

Project Budget By Task and BP

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Total Program Funding: $2,792,000 / 30 months

Planned Costs Fiscal Year	Fiscal Year	Performing Organization	Planned Costs
			Federal Share
1	FY2017	Laboratory	$246,046
2	FY2018	Laboratory	$1,178,391
3	FY2019	Laboratory	$1,061,031
2	FY2020	Laboratory	$306,532
		TOTAL	**2,792,000**

Budget Period 1 (BP1)	Costs
1. Project Management (BP1 & BP2)	$121,444
2. Solvent Physical Property Measurements (1-BEIPADIP-2-BOL)	$508,399
3. Solvent Synthesis (1-BEIPADIP-2-BOL)	$197,757
4. Initial Techno-Economic Projections	$74,492
5. Laboratory Continuous Flow System (LCFS) Redesign	$605,531
6. Initial CCSI² Engagement	$104,895
7. Initial Industry Outreach	$66,482
	Total BP1 budget $1,679,000
Budget Period 2 (BP2)	
8. Solvent Durability Measurements	$351,110
9. Laboratory Continuous Flow System Testing	$337,565
10. Final Techno-Economic Projections	$131,615
11. Data Needs for Future Process Scale-Up	$188,547
12. Final CCSI² Engagement	$75,888
13. Final Industry Outreach	$28,275
	Total BP2 Budget $1,113,000

Project Milestones

No.	Budget Period	Task/ Subtask	Milestone Description	Planned Completion	Verification Method
M1.1	1 & 2	1	Updated Project Management Plan	5/25/2017	Project Management Plan file
M1.2	1	1	Kickoff Meeting	9/15/2017	Presentation file
M1.3	1 & 2	1	Quarterly progress reports	30 days after end of each reporting period	Quarterly report file
M1.4	1	1	Go-No-Go Presentation at NETL	12/15/2018	Presentation file
M1.5	2	11	Delivery of final report - Final technical and economic feasibility study with recommendations of continuation for scale-up testing and industry hand off	Report 30 days after end of project completion,	Report and Presentation
M2.1	1	2	Solvent physical properties measured. k'g values comparable to MEA, VLE confirms 90% capture, ~70 ˚C reboiler drop in temperature using PSAR	9/30/2018	Report file
M3.1	1	3	1.5-2L solvent synthesized for testing. Synthetic costs of ~$15/kg of compound	10/31/2017	Notification to DOE & report file
M3.2	1	3	3-5L solvent synthesized for testing. Synthetic costs of ~$10/kg of compound	12/31/2018	Notification to DOE & report file
M4.1	1	4	Preliminary TEA projections show costs targets near $50/ton CO_2 with potential to reach $40/ton	3/31/2018	Notification to DOE & report file
M5.1	1	5	Continuous flow cart retrofitted and shaken down with optimal absorber and stripper configurations provided by CCSI[2]	12/31/2018	Presentation file
M8.1	2	8	Chemical degradation mechanisms quantified and any necessary mitigation strategies developed. Solvent lifetime and makeup rates quantified	9/29/2019	Notification to DOE & report file
M9.1	2	9	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	Notification to DOE & report file
M10.1	2	10	Final TEA completed with costs targets at or below $30/ton CO_2	12/31/2019	Notification to DOE & report file

Project Risk Matrix

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Description of Risk	Probability (Low, Moderate, High)	Impact (Low, Moderate, High)	Risk Management Mitigation and Response Strategies
Technical Risks:			
Solvent exhibits intolerance to SO_x, NO_2, O_2	Moderate	Moderate	Study mechanisms of degradation and investigate the use of chemical additives to minimize or retard degradation rate.
Costs of solvent are > $10/kg	Moderate	Low	Revise synthetic methodology until new synthetic routes meet the cost target
Poor water tolerance, e.g. bicarbonate precipitation or hydrolysis	Moderate	Moderate	Addition of chemical additives to minimize degradation. Test three alternate molecules for one derivative that can handle a 5-10 wt% water load with minimal amount of hydrolysis
Resource Risks:			
Key staff leave organization	Low	High	Prior to staff departure, identify replacement staff with required skillset.
Test equipment breaks down or is unavailable	Low	High	Build testing and maintenance schedule into testing plan
Chemical suppliers unable to provide starting reagents for synthesis	Moderate	High	Identify multiple chemical suppliers, or alternate synthetic methodologies for candidate molecule synthesis
Management Risks:			
Staff overcommitted	Low	Moderate	Use resource management tools
Scope creep	Low	Moderate	Notify DOE and reallocate project resources to meet deliverables and milestones.
Budget underestimation	Low	Moderate	Notify DOE and revise scope.

Project Deliverables

Quarterly and final reports will be submitted in accordance with NETL requirements.

Reporting:

- Finalized Project Management Plan
- Quarterly Progress Reports
- Fiscal year report
- Comprehensive Final Report
- Publications in scientific journals

Briefings and Technical Presentations

- Kick-off presentation
- Go no-go presentation
- Annual NETL CO_2 Technology Meetings
- $CCSI^2$ meetings
- DOCCSS workshops

Plans for Future Testing/Development/Commercialization

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- Disseminate all program findings via reports and publications
- Hand-off technology to an industrial partner
- Continued testing (if needed) with industrial partner

NATIONAL CARBON CAPTURE CENTER

CO_2 TECHNOLOGY CENTRE MONGSTAD

Acknowledgements

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

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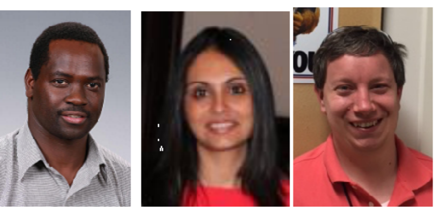
PNNL Team

Solvent Design / Chemical Durability / Synthesis & Scaleup



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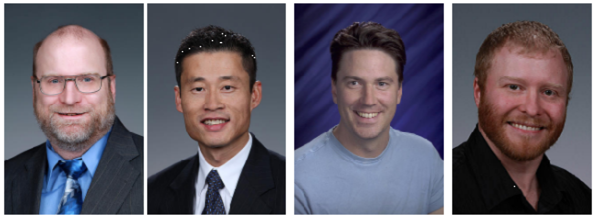

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Process Modeling Performance Projections

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CCSI[2] Carbon Capture Simulation for Industry Impact

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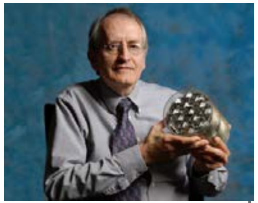

Professor Gary Rochelle