PARAMETRIC TESTING OF CO_2-BINDING ORGANIC LIQUIDS (CO_2BOLs) TO ENABLE INDUSTRY ADOPTION (FWP-76270)

[NETL/DOE Project Manager: Dustin Brown]

U.S. DEPARTMENT OF ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY
CARBON MANAGEMENT AND NATURAL GAS & OIL RESEARCH PROJECT REVIEW MEETING
VIRTUAL MEETINGS AUGUST 2 THROUGH AUGUST 31, 2021

Acknowledgment

Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

"This material is based upon work supported by the U.S. Department of Energy under Field Work Proposal FWP-76270."

Engineering-Scale Test of a Water-Lean Solvent for Post-Combustion Capture

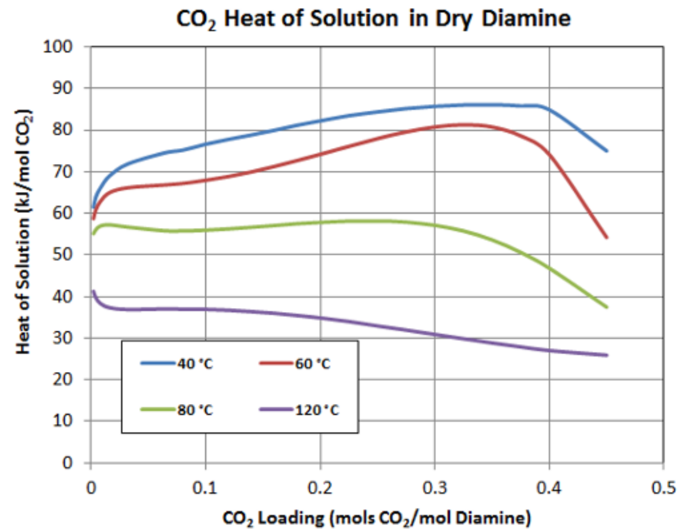
▶ DE-FE0031945

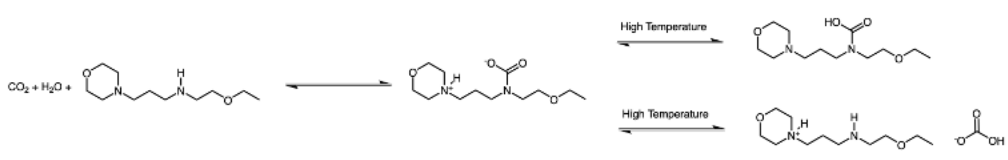
EEMPA can achieve low specific reboiler duties

The favorable thermal performance is attributable to

- The low water content (around 2 wt.% or less) meaning less water to vaporize
- A shift in the ionic character of the solvent with higher temperature, disfavoring the CO_2-bound ionic species

▪ SRDs down to 2.0 GJ/tonne have been observed in experiments. Cost-optimal designs for coal indicate 2.34 GJ/tonne is achievable.





Zheng et al. *Energy Environ. Sci.*, **2020**, *13*, 4106-4113.

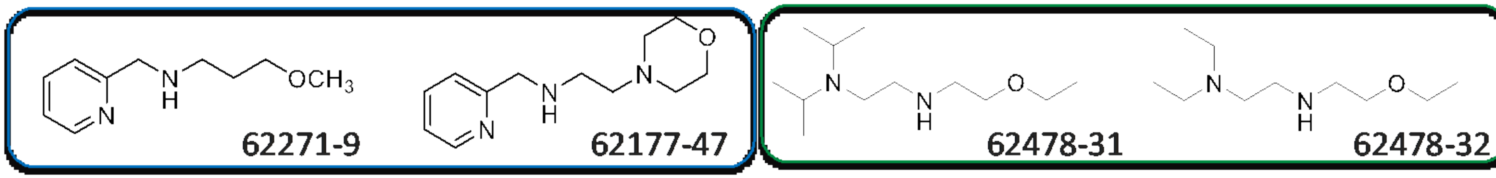
Jiang et al. *IJGHGC*, **2021**, *106*, *103279*.

Project Overview

Project Period: *5/1/2020-2/28/2022*

Funding: *$1,827,000*

Aminopyridines **Diamines**



Project Objectives:

- Provide critical data needed to project performance of three 3rd generation CO_2BOL single-component water-lean formulations (diamine, 2 aminopyridines)
- Measure essential physical and thermodynamic properties and demonstrate >90% capture of CO_2 on simulated flue gas for 40+ hours in steady-state operation
- Assess chemical durability of 3rd Generation CO_2BOL diamines and aminopyridines on simulated flue gas.
- Prime viable solvents for slip-stream testing and engage industrial partners for industry handoff.

Project Milestones

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

Completed dates underlined.

No.	BP	Task/ Subtask	Milestone Description	Initial Planned Completion
M1.1	1	1	Updated Project Management Plan.	6/1/2020 (completed)
M1.2	1	1	Go-No Go Presentation at NETL.	2/28/2021
M1.3	1	1	Delivery of final report to NETL	1/31/2022
M2.1	1	2	3-5L EEDIDA synthesized for testing. Synthetic costs of ~$10/kg of compound.	9/30/2020 (completed)
M3.1	1	3	EEDIDA kinetics and VLE measured. k'g values comparable to MEA, VLE confirms heat of solution between -75 to -85 kJ/mol (enabling 90% capture).	1/31/2021
M4.1	1	4	Continuous Flow Testing on EEDIDA completed. At least 40 hours of steady state 90% capture from simulated flue gas (15% CO2, 85 % N2 with SOx, NOx, O2) with and without PSAR.	2/28/2021
M4.2	1	4	Final TEA of EEDIDA completed with costs targets at or below $40/tonne CO2	2/28/2021

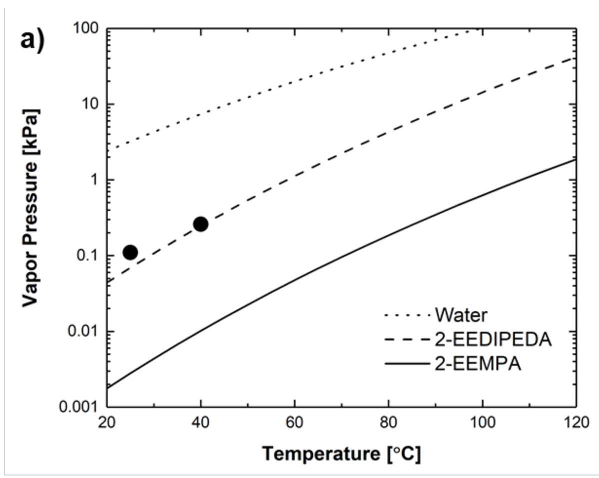
Success Criteria- BP1

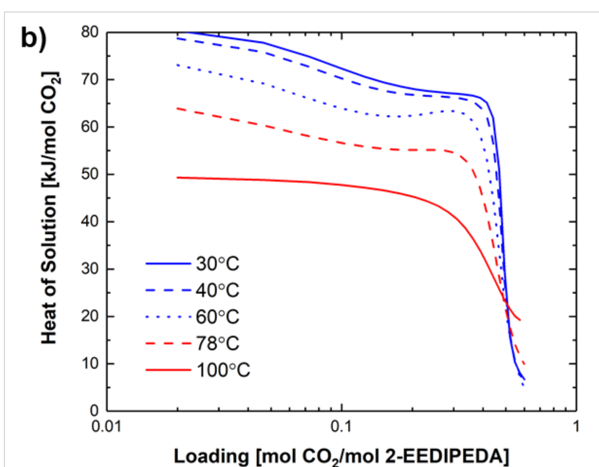
All criteria for BP1 were met by 2/28/2021.

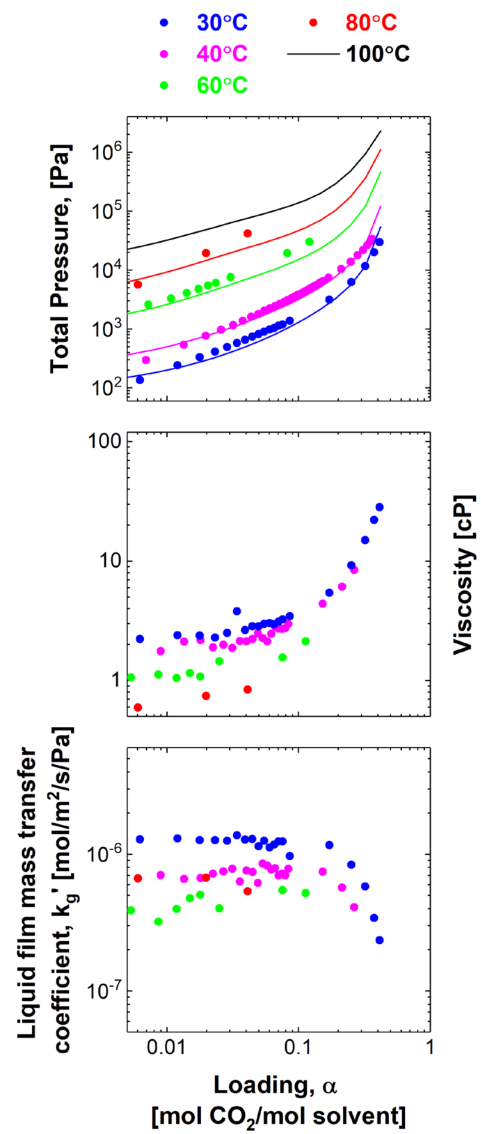
Date	Success Criteria
2/28/2021	Projected reboiler duty for EEDIDA in a simple stripper configuration is <2.0 GJ/tonne CO_2 or lower.
2/28/2021	Total costs of capture for EEDIDA are <$50/tonne CO_2, with potential to meet DOE's $40/tonne target in future efforts.
2/28/2021	Two new potential commercialization partners have been engaged to potentially partner on subsequent scale-up testing.

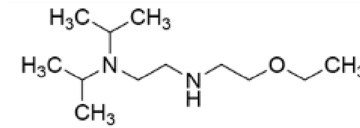
Physical Property Measurements

2-EEDIDA is comparable to 2-EEMPA, with lower viscosity and higher selectivity.









Barpaga et al. *In preparation*

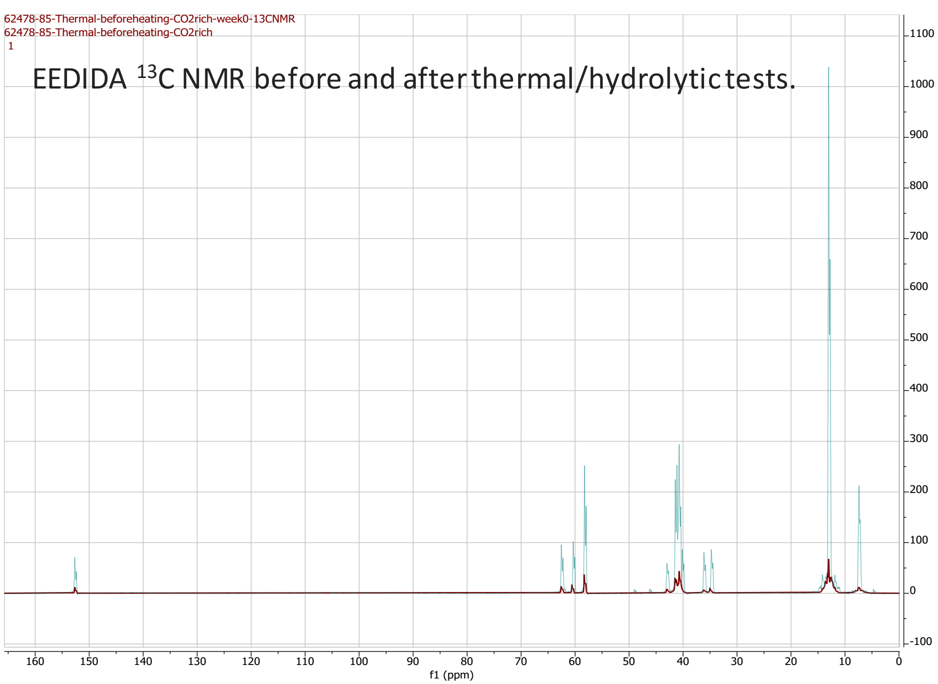
Chemical Durability Testing

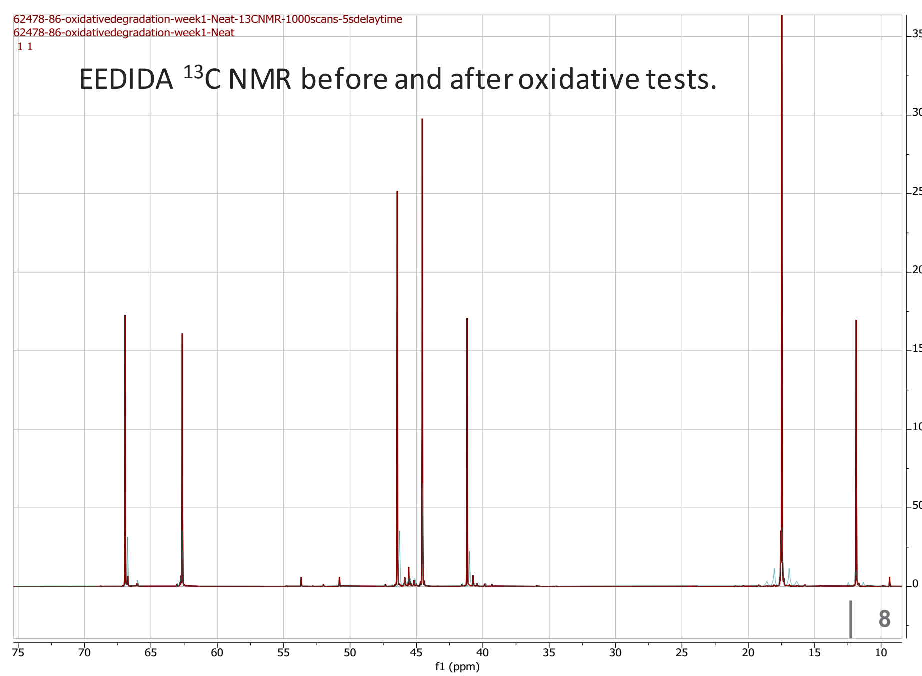
Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965

2-EEDIDA is durable under absorber and stripper conditions, comparable to 2-EEMPA.

- Hydrolysis tests at simulated stripper conditions: 5-weeks, 117°C, 5 wt% water, CO_2 saturated, in tubular reactors with periodic sample analysis.
- Oxidative degradation tests at simulated absorber conditions: 0.5 mol-CO_2/mol in autoclave, 55°C, 2% CO_2/air mixture gas, 3 weeks, with periodic liquid analysis.
- ^{13}C NMR, LC/MS and MS analysis suggests negligible degradation

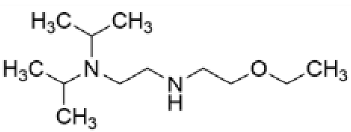


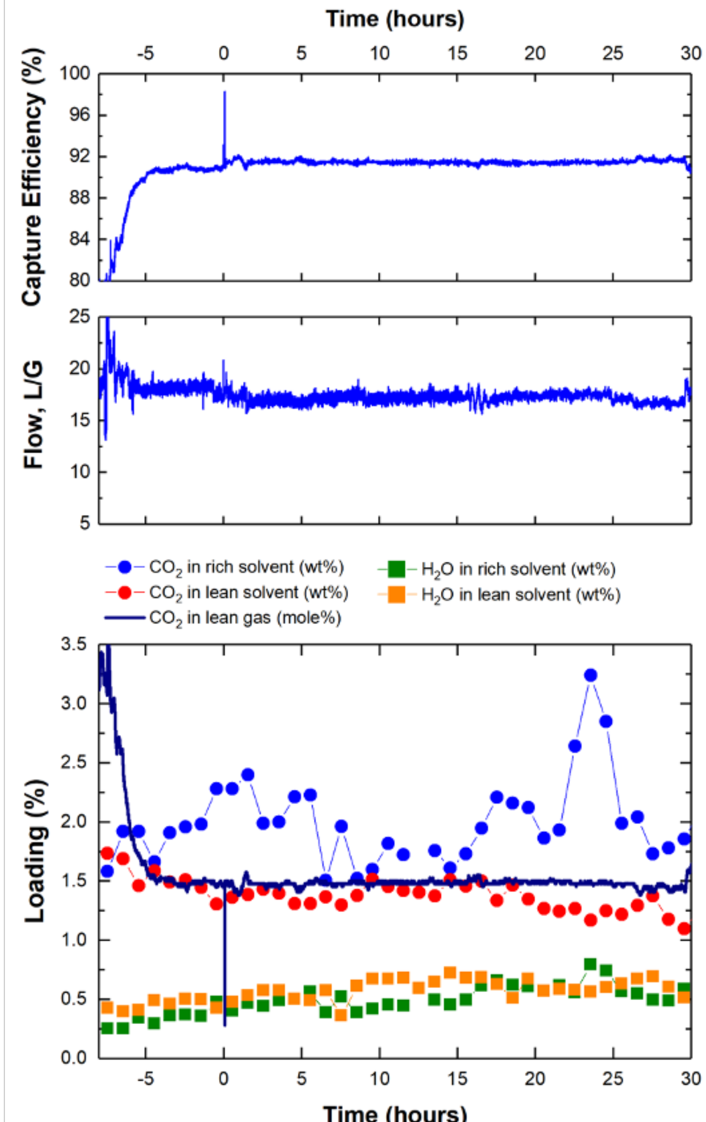


Lab-Scale Testing on Simulated Flue Gas

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

2-EEDIDA achieved 40 hours steady-state CO_2 capture with no foaming, aerosols or LLE.



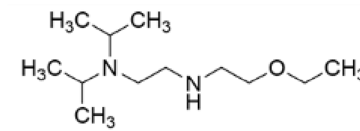


Barpaga et al. *In preparation*

Techno-Economic Analysis

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by **Battelle** *Since 1965*

2-EEDIDA is projected to be 20% cheaper than B12B Baseline, and $1.1/tonne cheaper than 2-EEMPA.*



Variable	MEA	Cansolv	2-EEMPA	2-EEDIDA		
NETL Reference	Case 12	Case B12B	Case B12B	Case B12B		
Configuration	SS	LVC	SS	TSF	SS	**TSF**
Lean Loading [mol CO_2 / mol solvent]	0.27	-	0.113	0.113	0.113	**0.113**
Rich Loading [mol CO_2/mol solvent]	0.50			0.328	0.328	**0.344**
Water Loading [wt%]	70	-	1.6	1.6	1.7	**1.7**
Regeneration Temp [°C]	115	-	96	98	98	**103**
Regeneration Pressure [bar]		1.98	1.98	2.32	5.2/2.3	**2.32**
Reboiler Duty [GJ_e/tonne CO_2]	3.55	2.48	2.35	2.36	2.22	**2.30**
Total Plant Cost [MM$, 2011]	-	632	530	497	505	**488**
Cost of Capture [$/tonne CO_2]	**-**	**58.3**	**49.1**	**47.1**	**47.7**	**46.6**

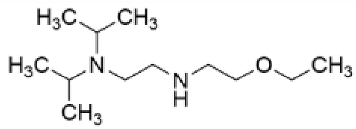
All costs are in 2012 dollars using NETL REV3 pricing.

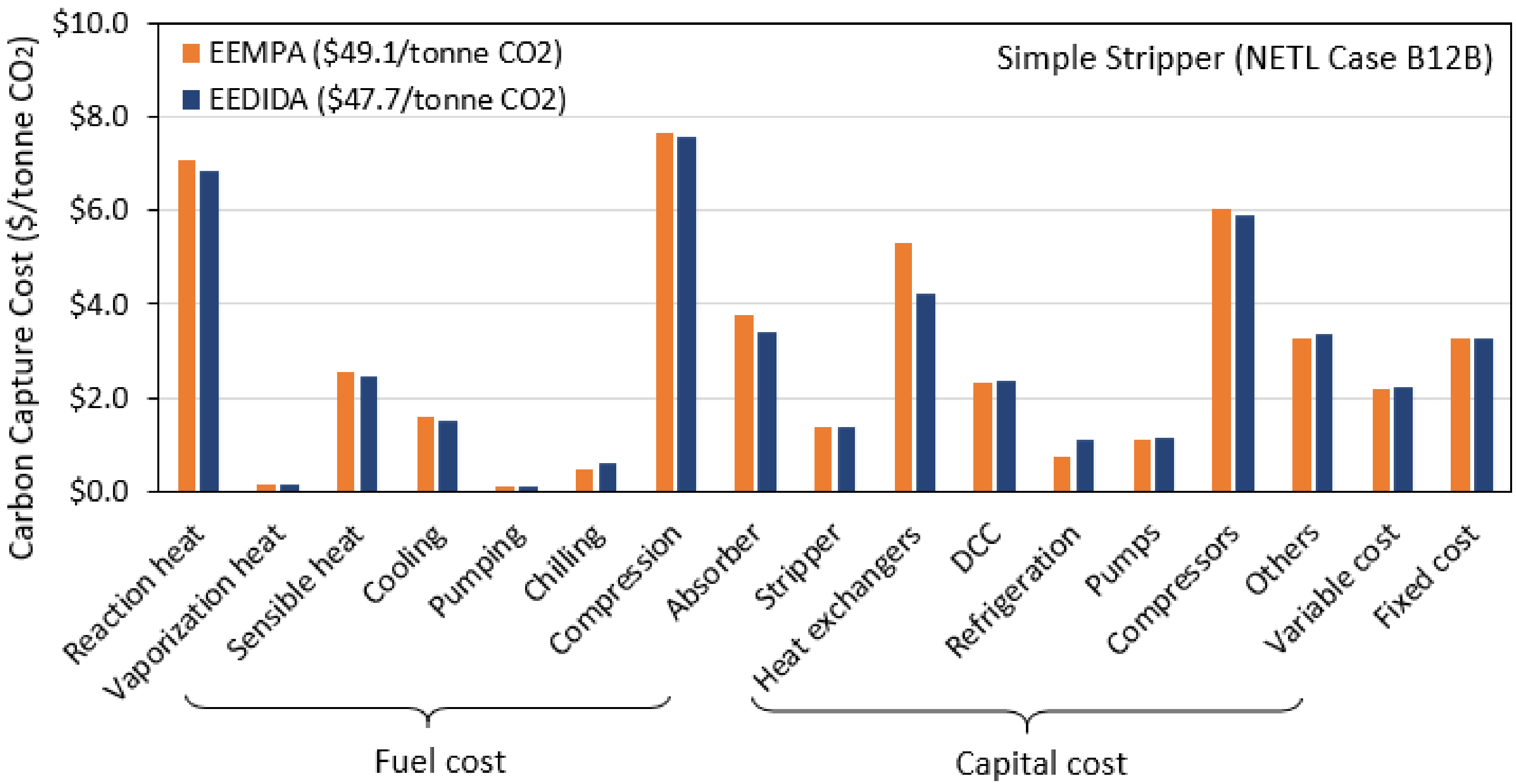
Barpaga et al. *In preparation*

Techno-Economic Comparison With 2-EEMPA

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

2-EEDIDA is $1.4/tonne cheaper than 2-EEMPA due to lower viscosity and higher selectivity.



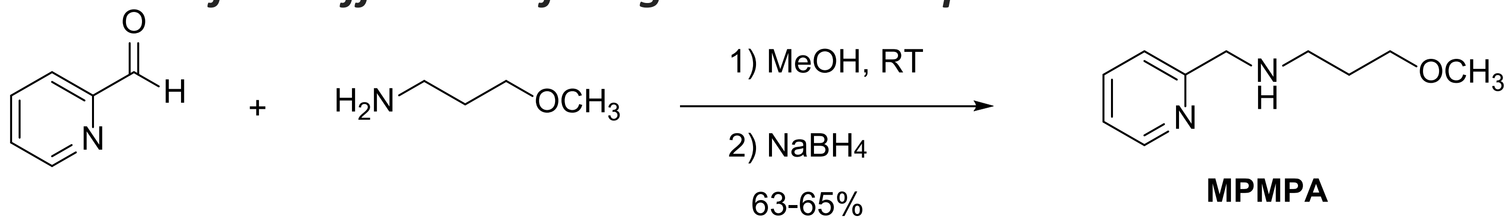


- Squeezing the lemon with respect to viscosity.

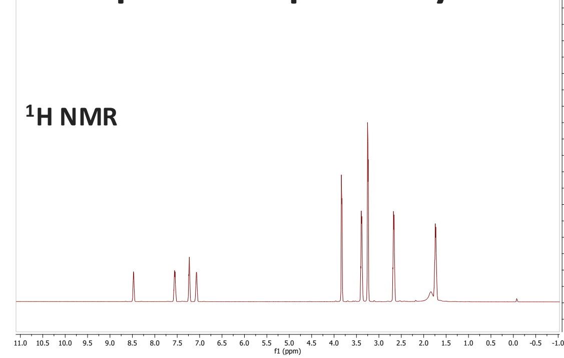
Barpaga et al. *In preparation*

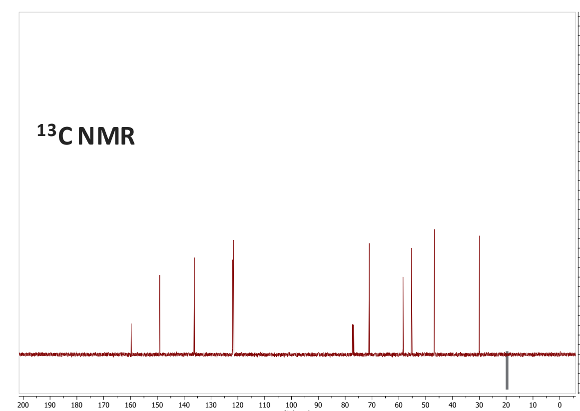
Synthesis of MPMPA solvent

MPMPA is made from off the shelf-reagents in a 1-step condensation.



Spectroscopic Analysis

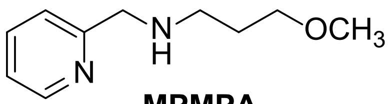




- Completed the synthesis of 3L of MPMPA solvent
- The estimated cost of MPMPA solvent production is ~ \$9/Kg
- MPMPA is stable up to 200 °C under vacuum distillation

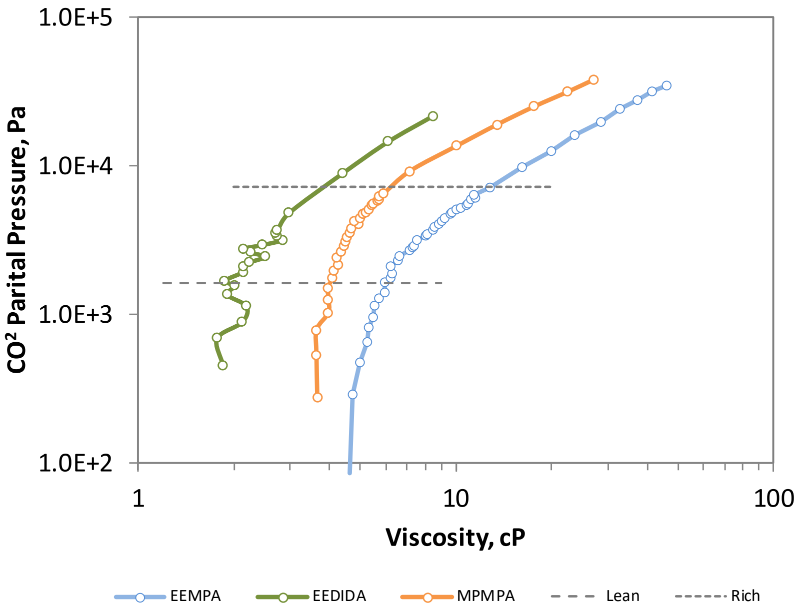
Physical Property Measurements

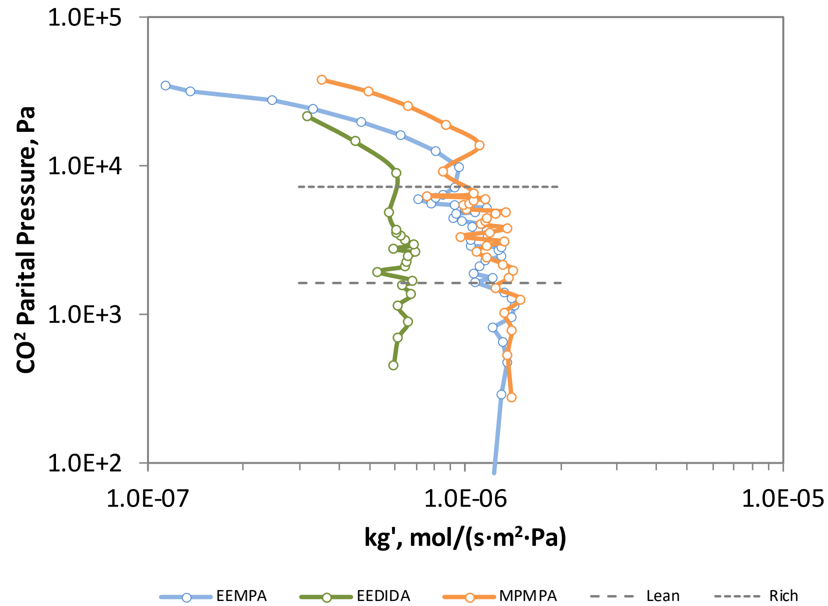
MPMPA has comparable properties to 2-EEMPA and 2-EEDIDA.



MPMPA

ΔH -71.6 to -78.0 kJ/mol
Vapor pressure <0.02 torr at 40 °C



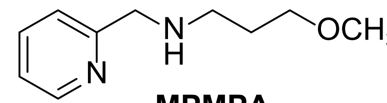


Barpaga et al. *In preparation*

Current and Future Work

Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

MPMPA is set to undergo thermal and oxidative stability and testing on WWC and LCFS.



MPMPA

Project Schedule and Major Tasks – BP2

Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

	BP-1								BP2													
	FY20					FY21												FY22				
	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F
Budget Period 2 (BP2)																						
1b. Project Management																						
5. Solvent Scale-up (AP: 1)																						
5.1 Develop solvent synthesis methodology with scale-up projections																						
5.2 Initial solvent scale-up production																						
5.3 Solvent physical property measurements (e.g. VP, flash point, density)																						
5.4 Solvent durability and chemical degradation assessment																						
6. Solvent Testing (AP: 1)																						
6.1 Vapor-liquid equilibrium, viscosity and other properties																						
6.2 Wetted-wall kinetics testing																						
6.3 Preliminary TEA																						
7. Laboratory Continuous Flow System Testing (AP: 1)																						
7.1 Parametric testing																						
7.2 Long duration testing on realistic flue gas																						
7.3 Data analysis and reporting																						
7.4 Final TEA																						
8. Solvent Scale-up (AP: 2)																						
8.1 Develop solvent synthesis methodology with scale-up projections																						
8.2 Initial solvent scale-up production																						
8.3 Solvent physical property measurements (e.g. VP, flash point, density)																						
8.4 Solvent durability and chemical degradation assessment																						
9. Solvent Testing (AP: 2)																						
9.1 Vapor-liquid equilibrium, viscosity and other properties																						
9.2 Wetted-wall kinetics testing																						
9.3 Preliminary TEA																						
10. Laboratory Continuous Flow System Testing (AP: 2)																						
10.1 Parametric testing																						
10.2 Long duration testing on realistic flue gas																						
10.3 Data analysis and reporting																						
10.4 Final TEA																						

Total - BP2

Conclusions and Future Work

Key Findings:

- 2-EEDIDA is a viable solvent for post-combustion capture
  - 20% cheaper than Case 12B baseline (CANSOLV)
  - \$1.4/tonne CO_2 cheaper than 2-EEMPA
  - Chemically durable

- MPMPA preliminary analysis suggests comparable properties as 2-EEMPA and 2-EEDIDA

Upcoming efforts:

- Full kinetics and continuous flow testing for MPMPA on simulated flue gas

- Update all pricing and TEA to REV4 (2018 \$)

Acknowledgements

PNNL Team

DOE/NETL PM: Dustin Brown


Charles Freeman


Yuan Jiang


Richard Zheng


Dushyant Barpaga


Greg Whyatt


Andy Zwoster

Parametric Testing
and Analysis
Process Modeling


David Heldebrant


Phillip Koech


Deepika Malhotra


Kat Grubel

Solvent Design
Synthesis & Scaleup
Chemical Durability