Universal Solvent Viscosity Reduction via Hydrogen Bonding Disruptors

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Project Overview

- Funding: $2,304,612
  - DOE: $1,843,690
  - Cost Share: $460,922

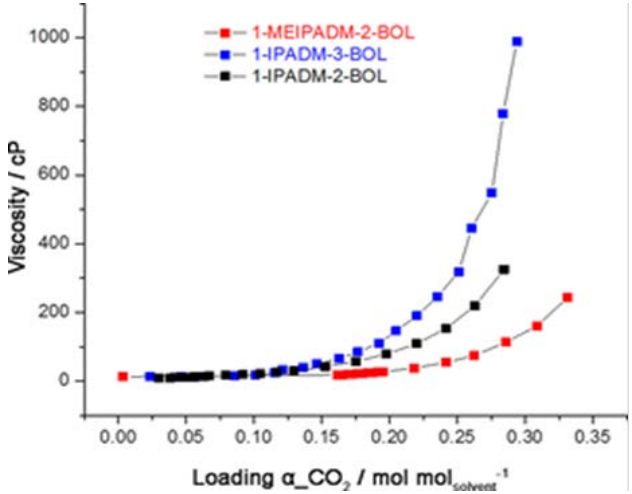
- Overall Project Performance Dates:
  - 10/01/2018 – 9/30/2021

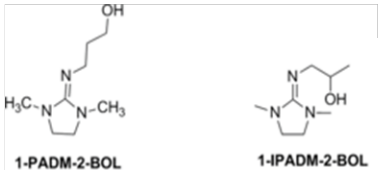
- Project Participants:
  - Liquid Ion Solutions (LIS)
  - Carnegie Mellon University (CMU)
  - Carbon Capture Scientific (CCS)

Project Objectives

- Computer simulation to understand the molecular interactions in non-aqueous CO_2 capture solvents.
- Synthesis and characterization of hydrogen bonding disrupter molecules with the specific goal of significantly reducing the viscosity of non-aqueous carbon capture solvents in the presence of CO_2.
- Proof-of-concept performance testing to demonstrate the effectiveness of hydrogen bonding disrupters in lowering viscosity.
- Optimization of hydrogen bonding disruptor chemical structure based on insights gained from computational modeling and experimental proof-of-concept studies.
- Demonstration of the effectiveness of the optimized hydrogen bonding disrupters in the presence of synthetic flue gas.

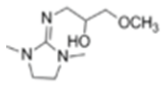
Technical Background - The Problem





1-PADM-2-BOL

1-IPADM-2-BOL



1-MEIPADM-2-BOL

Aqueous amine drawbacks:

- High energy cost for solvent regeneration
- Solvent loss due to evaporation
- Oxidative and thermal degradation in the adsorption-desorption cycles
- Corrosion problems

Non-aqueous amine drawbacks:

- High viscosity
  - Slower CO_2 uptake
  - Need more surface area (Larger equipment$$)

ChemSusChem **2017**, *10* (3), 636–642

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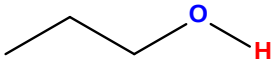
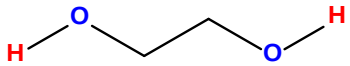
Effect of Hydrogen Bonding (HB) and Electrostatic (ES) on Viscosity



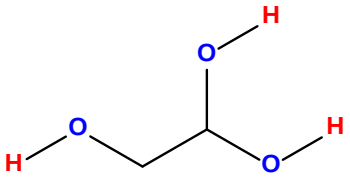
Molecular Weight: **60.10**

2 Cp @25°C



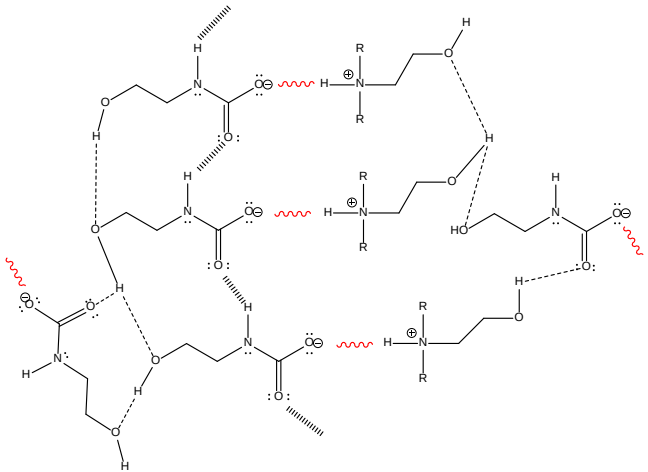
Molecular Weight: **62.07**

37 Cp @25°C



Molecular Weight: **78.07**

934 Cp @25°C



Hydrogen bonding and ionic bonding in a monoethanolamine based solvent

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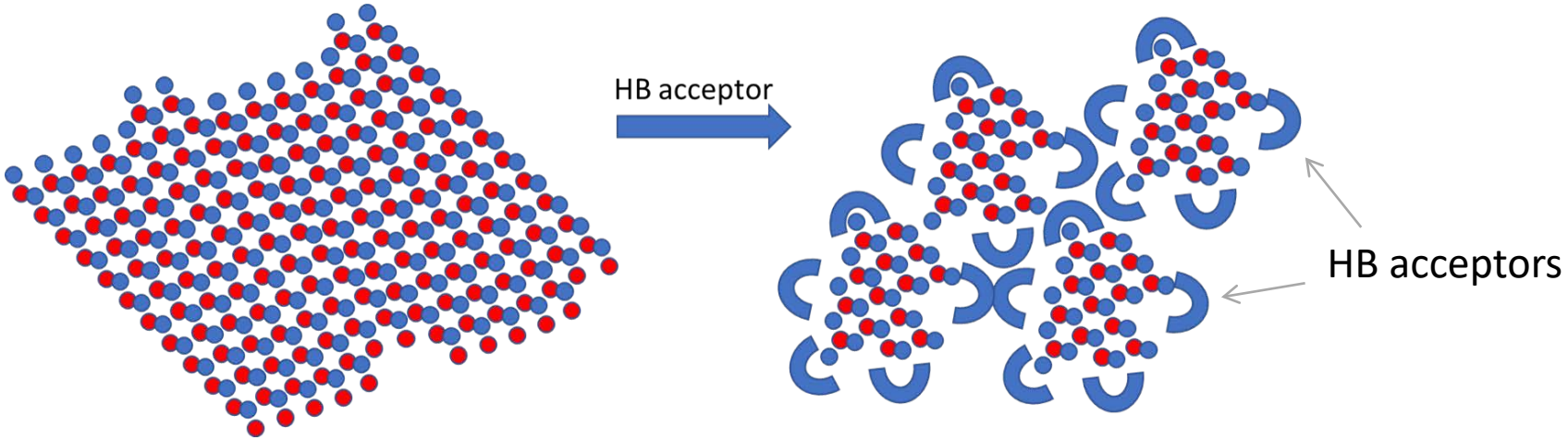
The Solution –Segmentation



Fully HB/ES bonded network

Brakeage of the network in smaller units

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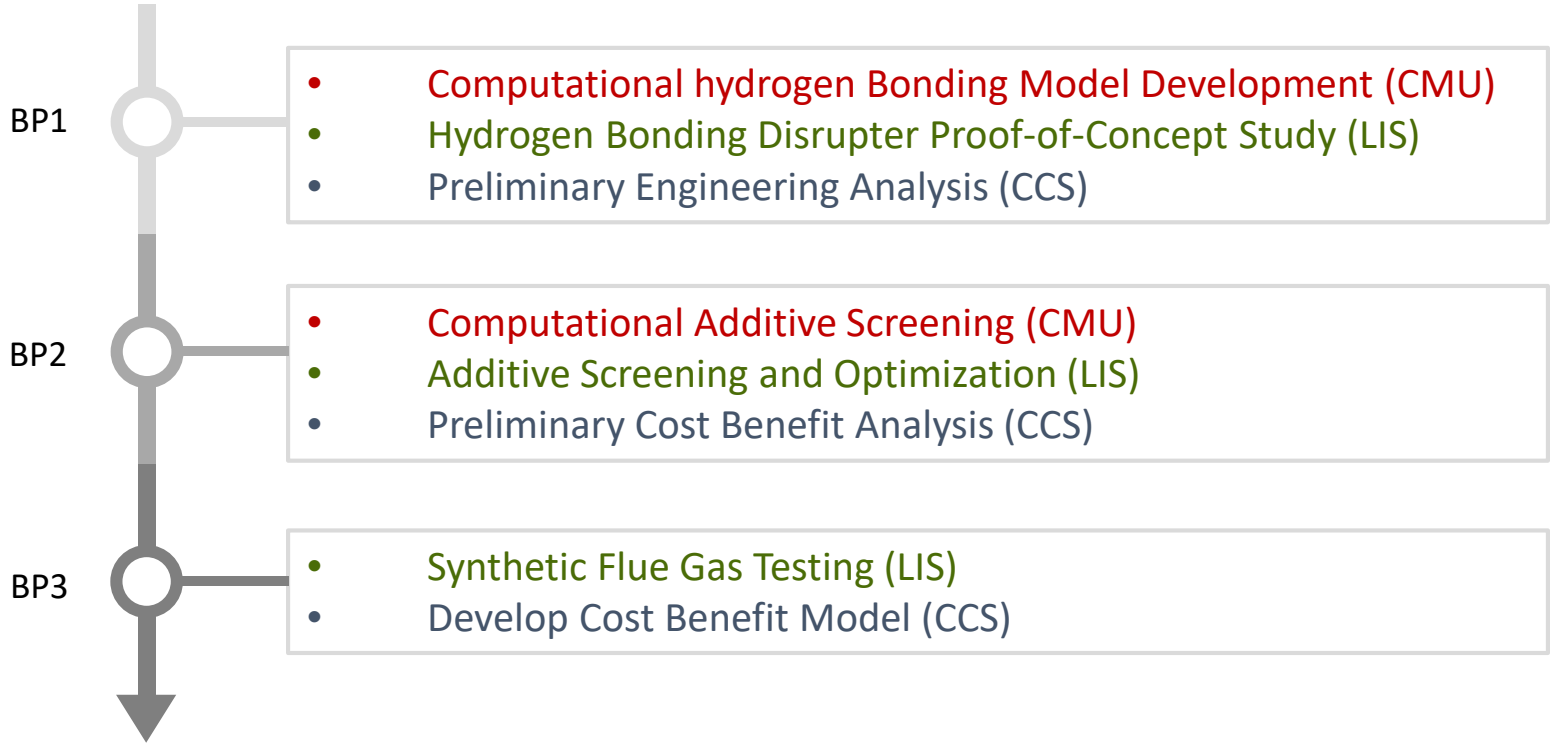
Project Schedule



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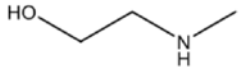
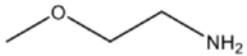
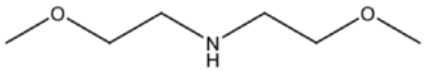
Research Progress

Task 2. Computational Hydrogen Bonding Model Development

Construction of Ab Initio Molecular Model

Chemical structure	Abbr.
	A1
	A2
	A3

Force field parameterization based on OPLS-AA force field with the aid of ab-initio calculations:

- Ab-initio calculations for amines and cations at MP2/6-31G(d,p) level, while those for anions were at MP2/6-31G++(d,p) level.
- Partial charges were fitted using CHELPG method.

Solvent	MD	Viscosity at 300K lit.	Viscosity at 298.15K exp.
A1	11.15	10.51	13.8
A2	0.59	0.66	0.6
A3	2.28	--	1.3

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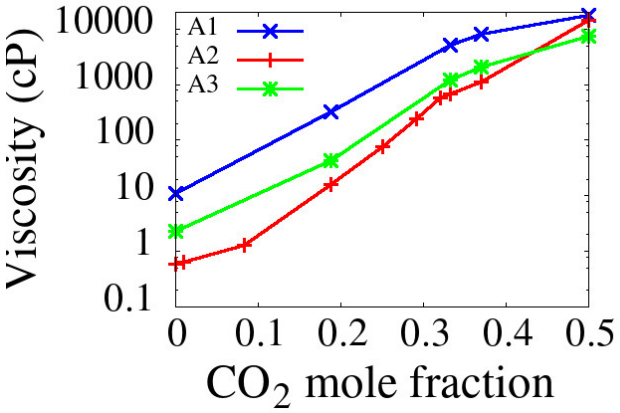
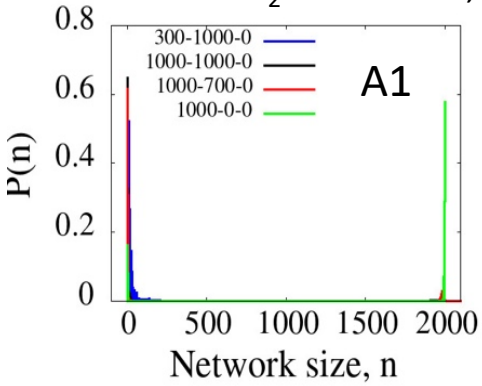
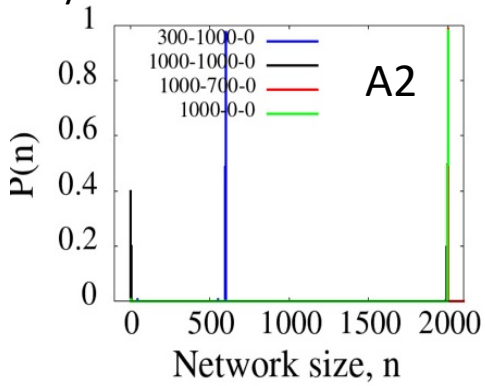
Simulation of Relationship between Hydrogen Bonding and Viscosity

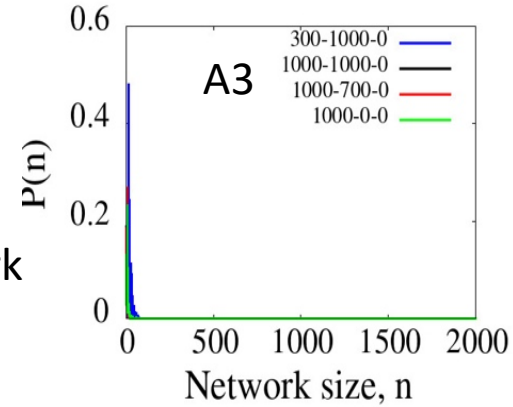


Viscosity vs CO_2 mole fraction
(= mol CO_2/mol total amine)
for A1, A2, and A3

Size distribution of "hydrogen-bonded" ion networks in CO_2-loaded A1 , A2 and A3 systems







Ions in A1 and A2 form essentially a single network
A3 forms many small networks.

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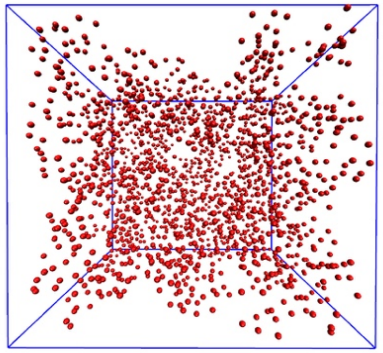
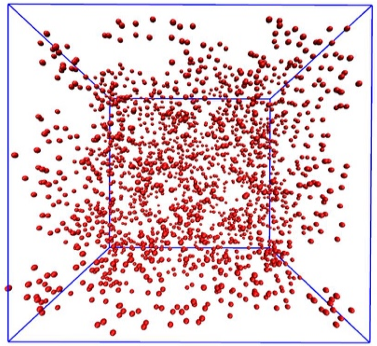
Quantitative Analysis of Co-solvent and Mixture Effects

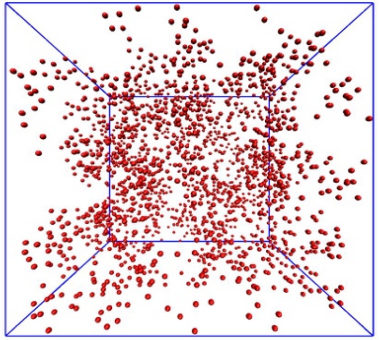
1000 A2 + 1000 ion pairs (CO_2 mole fraction = 0.333) + additives (DMSO)



No DMSO



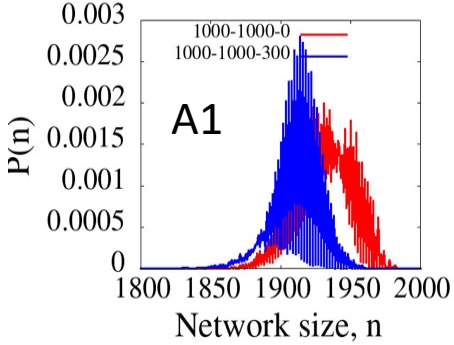
300 DMSO

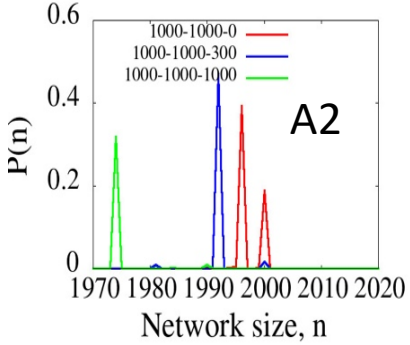


1000 DMSO

Only nitrogen atoms of ions are shown.

Size distribution of "hydrogen-bonded" ion networks in CO_2-loaded A1 and A2 systems





As DMSO are added, hydrogen-bonded ion network becomes "looser" and somewhat smaller

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Effects of Additives on System Viscosity

Type of amine	Mole fraction of adsorbed CO_2 vs total amine	Viscosity (cP)	Number of DMSO molecules	Number of water molecules	Viscosity with DMSO or water (cP)
A1	0.333	5148	300	0	3024
	0.370	8182	300	0	5278
	0.500	17641	300	0	8158
A2	0.188	16	300	0	14
	0250	78	300	0	44
	0.291	244	300	0	154
	0.333	684	300	0	377
	0.333	684	1000	0	175
	0.333	684	0	1300	742
	0.333	684	0	4000	207
	0.370	1134	300	0	957
	0.500	14370	300	0	6576
	0.500	14370	600	0	3309
A3	0.333	1197	300	0	568
	0.370	2029	300	0	1017
	0.500	7490	300	0	4010

- Viscosity increases as CO_2/amine ratio increases
- Both DMSO and water have similar effect on viscosity reduction
- The higher the additive %, the more viscosity reduction

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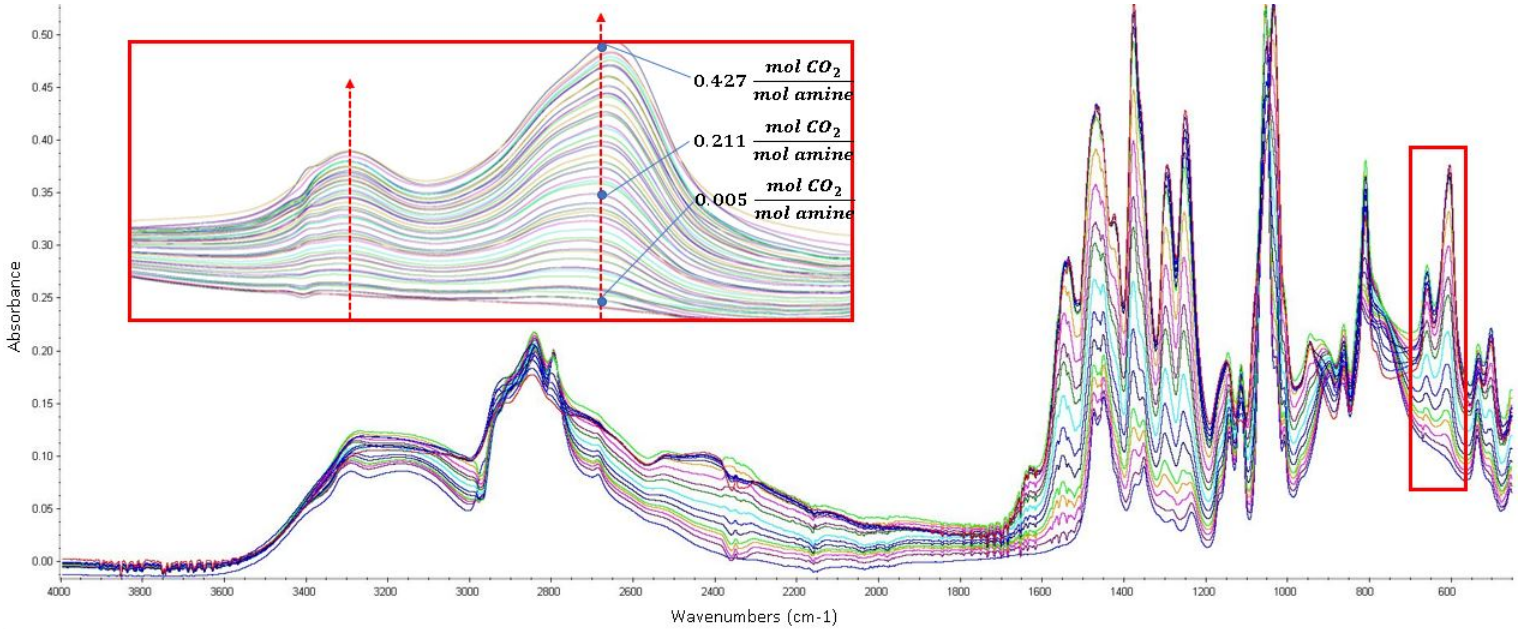
Task 3. Hydrogen Bonding Disruptor Proof-of-Concept Study

Baseline Solvent Testing



- Obtained quantitative correlation between CO_2 uptake and FT-IR spectra

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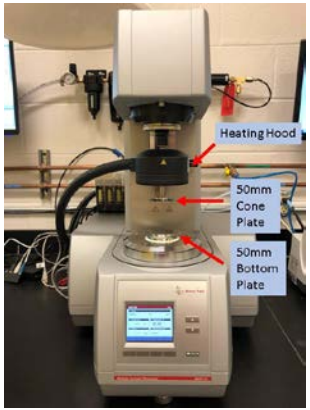
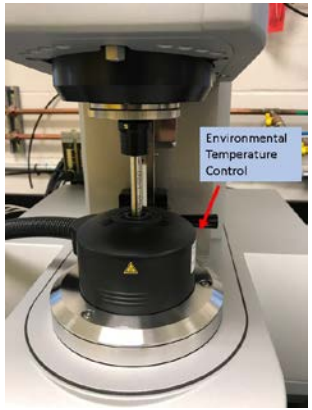
Task 3. Hydrogen Bonding Disruptor Proof-of-Concept Study cont'd

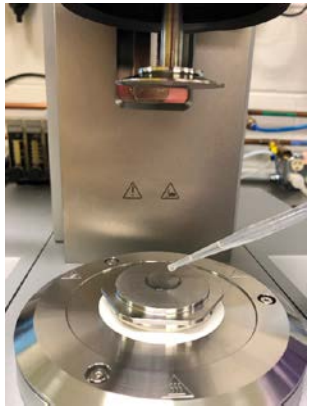
Initial Hydrogen Bonding Disruptor Synthesis

- Designed several classes of compounds with various molecular architectures and functionalities
- Prepared five promising candidates for viscosity testing.

Proof-of-Concept Viscosity Testing – Rheometer Setup







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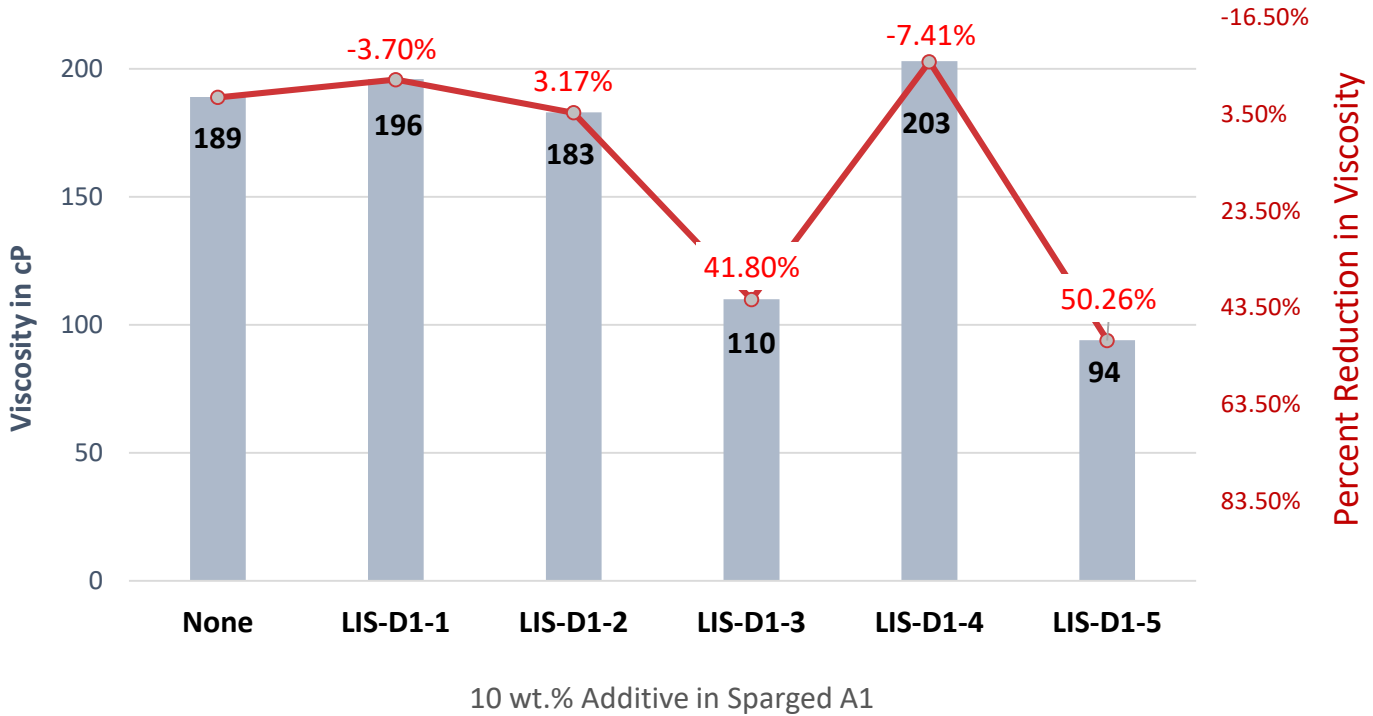
Task 3. Hydrogen Bonding Disruptor Proof-of-Concept Study cont'd

Effect of 10 wt.% additives on sparged A1



Task 3. Hydrogen Bonding Disruptor Proof-of-Concept Study cont'd

Effect of 10 wt.% LIS-D1-3 on sparged amines

Amine	CO_2 wt.%	Molar Ratio [CO_2/Amine]	Viscosity of Amine, cP	Viscosity of Amine + Additive, cP	% Reduction in Viscosity
A1	17.7	0.3021	189 ± 8	110 ± 1	41.8
A2	17.65	0.3012	22 ± 2	16 ± 1	27.3
A3	9.14	0.3021	4.8 ± 0.7	**1.8 ± 0.04**	62.5

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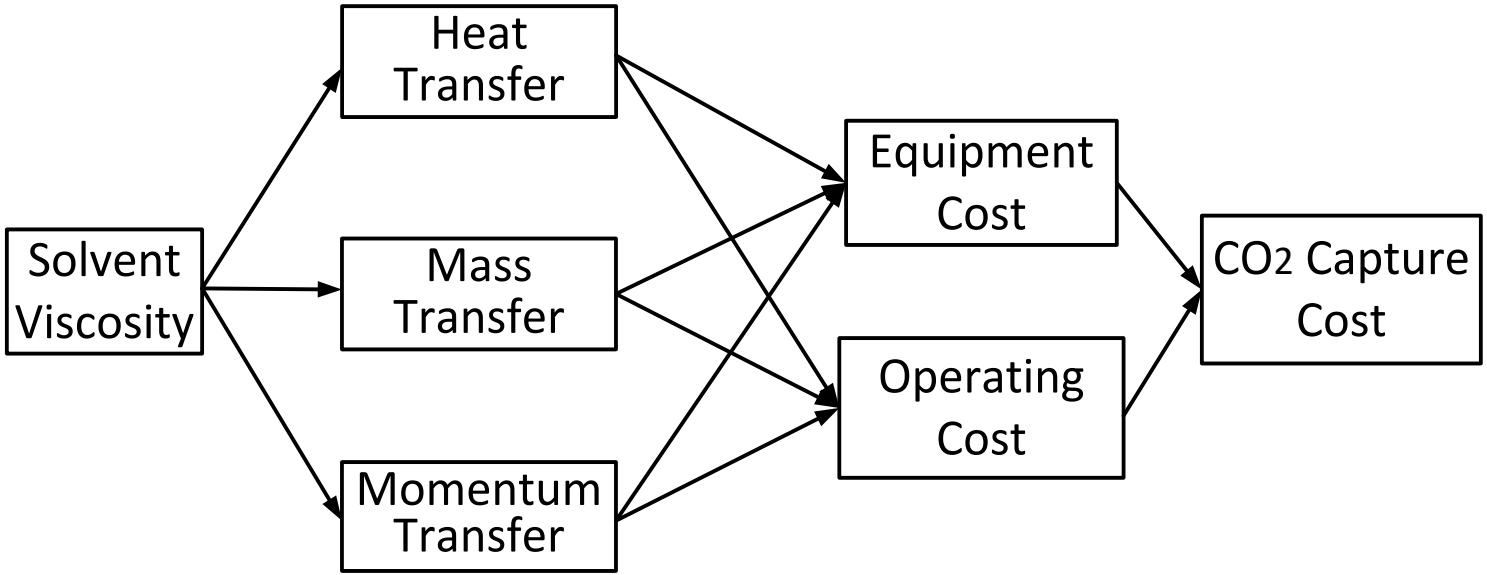
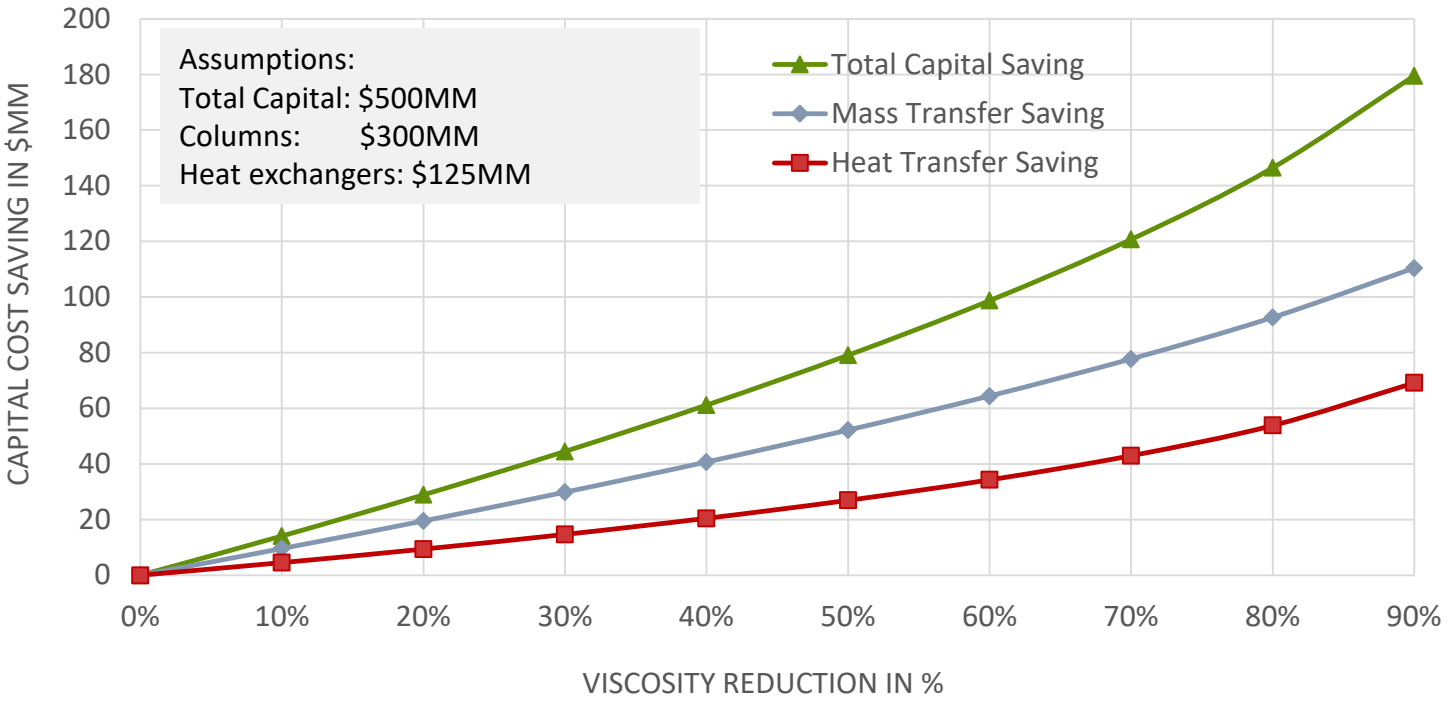
Task 4. Investigation of Impacts of Viscosity on Solvent Based CO_2 Capture Processes

Overall Approach



Task 4. Investigation of Impacts of Viscosity on Solvent Based CO_2 Capture Processes cont'd

Obtained Viscosity Impact on Total Equipment Cost



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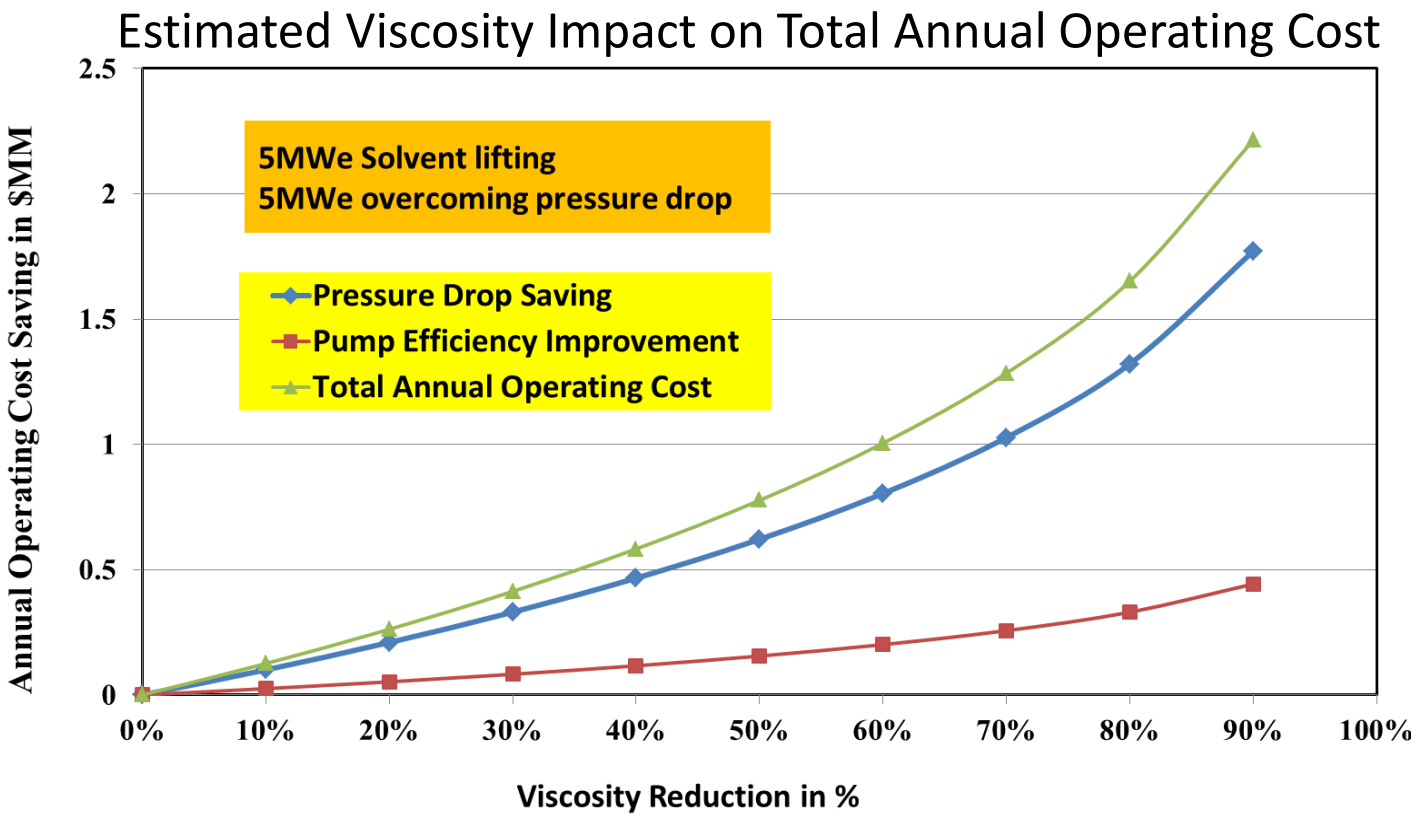
Task 4. Investigation of Impacts of Viscosity on Solvent Based CO_2 Capture Processes cont'd



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Conclusions and Future Plan

- Computational study gave insights on hydrogen bonding in the model solvents, viscosity at various CO_2 level, and additive effect on viscosity reduction.
- Additives LIS-D1-3 and LIS-D1-5 showed 40-50 % viscosity reduction on all model amines.
- LIS-D1-3/A3 system showed viscosity around 2 cP, demonstrating the potential feasibility of the additive approach.
- Preliminary engineering analysis revealed that a 50% reduction in solvent viscosity will reduce total equipment cost of an absorption/stripping based process by 15%.
- In the process of designing and preparing Gen2 additives based on the insights gained from BP1 research.

Acknowledgement and Disclaimer

Acknowledgment: "This material is based upon work supported by the Department of Energy under Award Number DE-FE0031629."

Thank you!

Any Questions?

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