Universal Solvent Viscosity Reduction via Hydrogen Bonding Disruptors

DOE Award Number: FE0031629
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Carbon Management and Oil and Gas Research Project Review Meeting
August 16, 2021
Materials Innovation at RoCo Global

Liquid Ion Solutions LLC rebranded to RoCo Global in 2020. It is an advanced materials company that develops innovative materials technologies to solve global environmental issues.
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 dba RoCo Global
  • Carnegie Mellon University
  • Carbon Capture Scientific
Overall Objectives

The project goal is to develop additives capable of decreasing viscosity of water-lean solvents for post-combustion capture.

The project objectives includes:

1. Perform and develop computer simulations to elucidate molecular interaction of various functionalities and how they impact viscosity.
2. Design, synthesize and perform testing of additives to reduce CO$_2$ capture solvent viscosity on model solvent systems.
3. Optimize and formulate additive-solvent systems for CO$_2$ capture.
4. Perform testing on the formulated model solvent in the presence of synthetic flue gas and quantify the impact and benchmark against commercially relevant solvent.
Water-lean Solvents – Opportunities and Challenges

<table>
<thead>
<tr>
<th></th>
<th>NETL Case 10 (MEA)</th>
<th>Water-lean solvents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estimated reboiler duty (Btu/lb CO₂)</td>
<td>1520</td>
<td>753-1100</td>
</tr>
<tr>
<td>Net plant efficiency (HHV)</td>
<td>25.4%</td>
<td>27.5-32.5%</td>
</tr>
<tr>
<td>Cost per tonne CO₂ capture (USD)</td>
<td>60</td>
<td>39-63</td>
</tr>
</tbody>
</table>

Viscosity as a function of CO₂ loading for a water-lean silylamine.

Solvent viscosity coupled with CO₂ capture capacity has a major impact on overall capture cost.

RoCo’s Additive Approach to Reduce Viscosity

RoCo additive breaks long-range hydrogen bonding and electrostatic interactions into smaller segments. The additive molecules have very low cohesive energy. This results in significant reduction in viscosity upon mixing with commercial amines.

Hydrogen bonded network
High viscosity

Segmentation of hydrogen bonded network
Low viscosity
Project Scope and Schedule

Budget Period 1
10/1/2018-9/30/2019

- Computational hydrogen Bonding Model Development
- Hydrogen Bonding Disrupter Proof-of-Concept Study
- Preliminary Engineering Analysis

Budget Period 2
10/1/2019-9/30/2020

- Computational Additive Screening
- Additive Screening and Optimization
- Preliminary Cost Benefit Analysis

Budget Period 3
10/1/2020-9/30/2021

- Synthetic Flue Gas Testing
- Develop Cost Benefit Model
BP1 Accomplishments

- Computational study gave insights on hydrogen bonding in the model solvents, viscosity at various CO$_2$ level, and additive effect on viscosity reduction.
- Proof-of-concept study demonstrated additives’ effectiveness on viscosity reduction.
- Preliminary engineering analysis showed a 50% reduction in viscosity will potentially save capital cost by about 16% and achieve $3.8/tonne CO$_2$ in capture cost saving without considering additive cost.

A1 and A2 rich samples contained ca. 18 wt% CO$_2$, A3 rich samples contained 9 wt% CO$_2$.
BP2 – Computational Additive Screening

- Computational design of additives
- Simulation of the effect of additives on viscosity, exploring 7 prototype additives with various functionalities and molecular structures
- Qualitative comparison between simulation and experimental results revealed similar trends in viscosity reduction among different additives, demonstrating the effectiveness of computational screening.

Insights gained from simulation study
- Important factors: large van der Waals volume; good flexibility; weak hydrogen-bond accepting power.
- Recommended 3 specific additives for experiment.
BP2 – Experimental Additives Development

- Additive screening exploring 7 functionalities and 3 molecular structures
- Additive optimization (loading and combination effect)

RoCo developed proprietary viscosity-reducing additives that can reduce viscosities of model amine solvents up to 50% upon CO₂ loading.
BP2 – Preliminary Cost Benefit Analysis

• Net benefit generated from adding viscosity-reducing agent (additive) into the solvent is significant.

• Additive approach significantly exceeds the targeted success criteria of $1/tonne CO₂ captured.

• The cost of additive compared to the benefit is insignificant.

• Based on this analysis, the cost of the additive is not important. The net benefit for the tested additives is directly correlated with the viscosity reduction magnitude. It means that the focus should be on how much the viscosity of a solvent can be reduced by this approach.
BP3 – Synthetic Flue Gas Study

Testing methods development and baseline testing
BP3 – Synthetic Flue Gas Study – cont’d

RoCo lab-scale testing unit

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Gas flow rate</td>
<td>Various: 1-11 ±0.1 SLPM</td>
</tr>
<tr>
<td>CO$_2$ in gas composition</td>
<td>4±0.5; or 15±0.5 vol%</td>
</tr>
<tr>
<td>Solvent flow rate</td>
<td>Various: 5-30±1 mL/min</td>
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<tr>
<td>Absorber temperature</td>
<td>40±5 °C</td>
</tr>
<tr>
<td>Stripper temperature</td>
<td>Various: 90-120±5 °C</td>
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</table>
Absorption tests

Absorption runs of an amine-additive solvent achieved up to 95% capture efficiency under simulated flue gas containing 15 vol% CO₂. We observed a viscosity of less than 5 cP with CO₂ uptake of ~4.8 wt% for rich solvent samples during these tests.
Future Plans

Remainder of this project:
• Steady state test (50 h) to evaluate solvent stability – in progress
• Refined cost benefit analysis – in progress

Next project:
• 3rd Generation, high performance, water-lean solvents for carbon capture (SBIR Phase I, Award # DE-SC0021827)

Exploring collaboration opportunities for scaling-up and commercialization
Summary

• The team conducted computational simulations on additive molecules with various functionalities and molecular structures for their effect on viscosity, showing good agreement with experimental results.

• We developed viscosity-reducing additives that can reduce viscosities of model amine solvents up to 50% upon CO\textsubscript{2} loading.

• Absorption runs of an amine-additive solvent achieved up to 95% capture efficiency under simulated flue gas containing 15 vol% CO\textsubscript{2}. We observed a viscosity of less than 5 cP with CO\textsubscript{2} uptake of ~4.8 wt% for rich solvent samples during these tests.

• Preliminary engineering analysis showed a 50% reduction in viscosity will potentially save capital cost by about 16% and achieve $3.8/tonne CO\textsubscript{2} in capture cost savings without considering additive cost.

• Cost benefit analysis showed that the net benefit generated from adding viscosity-reducing agent into the CO\textsubscript{2} capture solvent is significant, and the cost of an additive itself compared to the benefit is relatively insignificant.
Acknowledgment and Disclaimer

• This material is based upon work supported by the Department of Energy under Award Number DE-FE0031629

• DOE Program Manager: Katharina Daniels and Andrew Jones

• Project partners:

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Thank you!

Any Questions?
Appendix
Liquid Ion Solutions LLC (dba RoCo Global)
- Project management and planning
- Hydrogen bond disrupter proof-of-concept study
- Additive screening and optimization
- Synthetic flue gas study

Carnegie Mellon University
- Computational hydrogen bonding model development
- Computational additive screening

Carbon Capture Scientific LLC
- Preliminary engineering analysis
- Preliminary cost benefit analysis
- Develop cost benefit model
Gantt Chart

<table>
<thead>
<tr>
<th>Task Name</th>
<th>2018</th>
<th>2019</th>
<th>2020</th>
<th>2021</th>
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<td>Q4</td>
<td>Q1</td>
<td>Q2</td>
<td>Q3</td>
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<td>Task 1.0 – Project Management and Planning</td>
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<td>Task 2.0 – Computational Hydrogen Bonding Model Development</td>
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<td>Task 7.0 – Preliminary Cost Benefit Analysis</td>
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<td>Task 8.0 – Synthetic Flue Gas Study</td>
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<td>Task 9.0 – Develop Cost Benefit Model</td>
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- Milestones
- Completed
- In progress