Project Kickoff Meeting

Universal Solvent Viscosity Reduction via Hydrogen Bonding Disruptors

Liquid Ion Solutions

Carnegie Mellon University

CCS
CARBON CAPTURE SCIENTIFIC LLC

Project Objectives

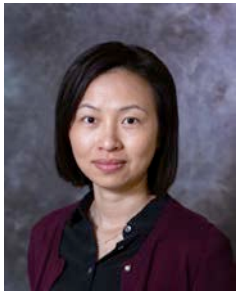
- Computer simulation to understand the molecular interactions in non-aqueous CO_2 capture solvents.
- Synthesis and characterization of hydrogen bonding disrupter molecules with the specific goal of significantly reducing the viscosity of non-aqueous carbon capture solvents in the presence of CO_2.
- 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.

Liquid Ion Solutions

LIS Team

Dr. Xu Zhou – Principal Investigator

- Experienced chemist
- Strong background in material development for carbon capture



Professor Hunaid Nulwala

- Experienced chemist with experience in industry, government, and academia
- Strong background in polymers, ionic liquids, gas separations
- Founder of two technology companies
- 50+ publications and 16+ patents and applications in material development

Dr. David Luebke

- Chemical engineer specializing in carbon capture
- Membrane scientist with experience designing, constructing and operating performance equipment
- Broad knowledge of carbon capture system

Liquid Ion Solutions

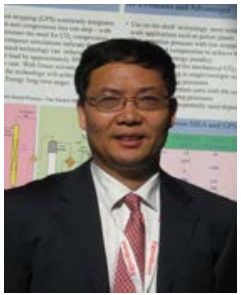
CMU Team

Carnegie Mellon University

Professor Hyung J. Kim

- Renowned scholar in the theoretical and computational field (100+ publications)
- Strong background in theoretical and computational analysis of chemical processes and related transport phenomena in solution, in nano-environments and at interfaces

CCS Team



CCS CARBON CAPTURE SCIENTIFIC LLC

Dr. Scott Chen

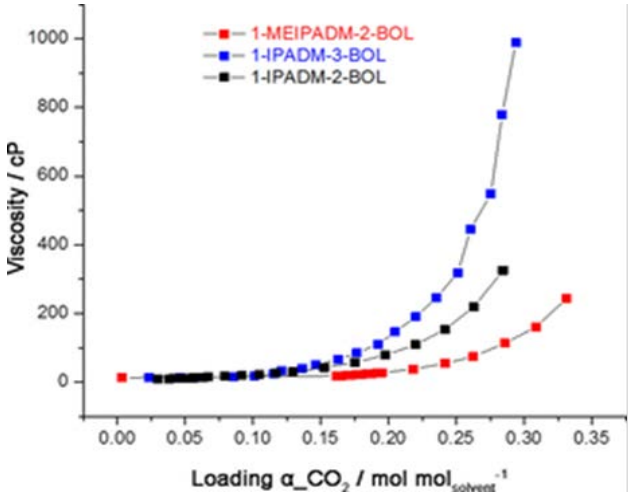
- Experienced chemical engineer
- Strong background in separation processes and thermodynamics
- Founder of Carbon Capture Scientific, LLC

Liquid Ion Solutions

Technical Approach

Liquid Ion Solutions

The Problem



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

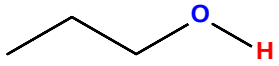
Non-aqueous amine drawbacks:

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

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

Liquid Ion Solutions

Effect of Hydrogen Bonding (HB) on Viscosity

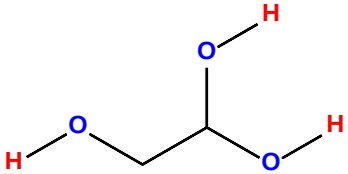


Molecular Weight: **60.10**

2 Cp @25°C

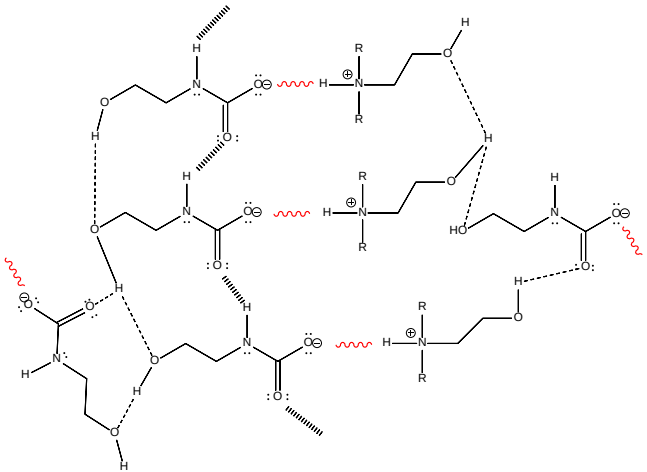
Molecular Weight: **62.07**

37 Cp @25°C



Molecular Weight: **78.07**

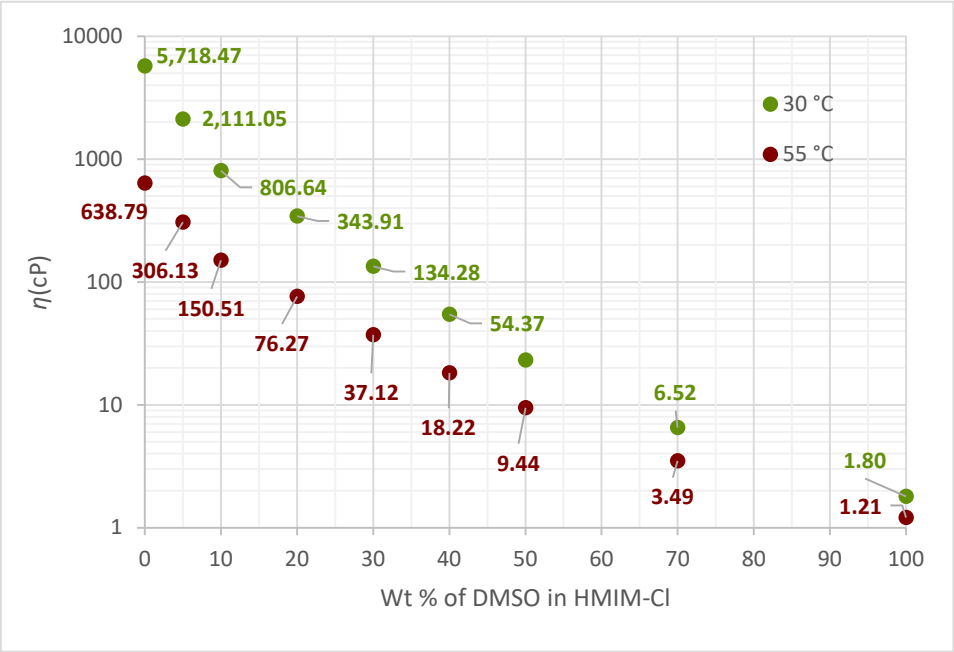
934 Cp @25°C



Hydrogen bonding and ionic bonding in a monoethanolamine based solvent

Liquid Ion Solutions

Additive Effect on Viscosity



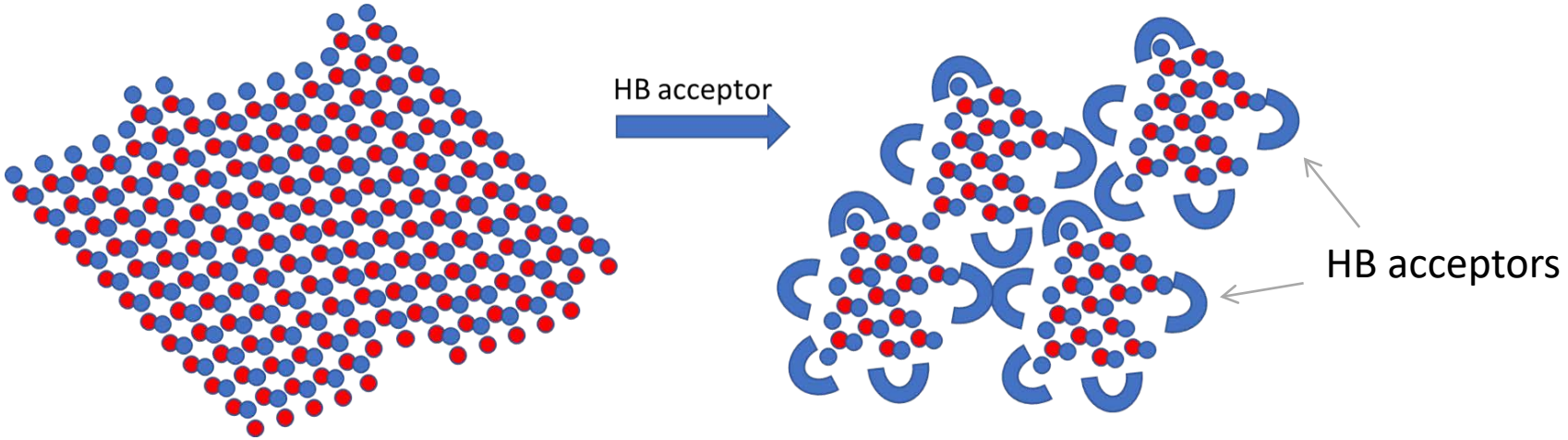
Viscosity effect of additions of DMSO on HMIM-Cl

5% DMSO to HMIM-Cl results in a 60% reduction in viscosity

J. Chem. Thermodyn. 2017, 113, 358.

Liquid Ion Solutions

The Solution – HB segmentation



Fully HB bonded network

Brakeage of the HB network

Liquid Ion Solutions

Tasks for Budget Period 1

Task 2.0 – Computational Hydrogen Bonding Model Development

- 2.1 – Construction of Ab Initio Molecular Model
- 2.2 – Simulation of Relationship between Hydrogen Bonding and Viscosity
- 2.3 – Quantitative Analysis of Co-solvent and Mixture Effects
- 2.4 – Guidance in Selection of Hydrogen Bonding Disrupters

Task 3.0 – Hydrogen Bonding Disrupter Proof-of-Concept Study

- 3.1 – Baseline Solvent Testing
- 3.2 – Initial Hydrogen Bonding Disruptor Synthesis
- 3.3. Proof-of-Concept Viscosity Testing

Task 4.0 – Preliminary Engineering Analysis

- 4.1 – Literature Review on the Impact of Viscosity
- 4.2 – Quantitative Assessment of Impact on Equipment Costs
- 4.3 – Quantitative Assessment of Impact on Operating Costs
- 4.4 – Sensitivity Analysis

Liquid Ion Solutions

Tasks for Budget Period 2

Task 5.0 – Computational Additive Screening

- 5.1 – Computational Design of Hydrogen Bonding Disruptors
- 5.2 – Simulation of the Effect of Additives on Viscosity
- 5.3 – Incorporation of Experimental Results

Task 6.0 – Additive Screening and Optimization

- 6.1 – Additive Structure Optimization and Synthesis
- 6.2 – Additive Loading Optimization Study

Task 7.0 – Preliminary Cost Benefit Analysis

- 7.1 – Experimental Data Review and Cost Estimation
- 7.2 – Preliminary Cost Benefit Analysis with Selected Additives

Liquid Ion Solutions

Tasks for Budget Period 3

Task 8.0 – Synthetic Flue Gas Study

- 8.1 – Synthetic Flue Gas Testing
- 8.2 – Cycle Testing for Evaluation of Degradation Products

Task 9.0 – Develop Cost Benefit Model

- 9.1 – Cost Benefit Analysis Revision
- 9.2 – Additive Sensitivity Analysis

Liquid Ion Solutions

Risk Management

Description of Risk	Probability (Low, Moderate, High)	Impact (Low, Moderate, High)	Risk Management Mitigation and Response Strategies
Technical Risks			
Additives do not significantly impact viscosity.	Low	High	Based on the proven correlation of solvent viscosity to hydrogen bonding network formation and the effectiveness of additives for control of viscosity in other applications, it is unlikely that the additives will be ineffective. Efforts will be made to identify this problem early in the project. If it occurs, different types of additives will be substituted.
Additives reduce solvent capacity.	Moderate	High	The small amount of additive required to break up hydrogen bonding networks should be insufficient to cause an appreciable decrease in capacity. If the capacity reduction is found to be significant, a different class of additives will be substituted.
Flue gas contaminants damage or deactivate additives.	Low	High	The additives may interact with SO_2, but those interactions should be less strong than with most solvent species. As a result, the effect of contaminants on the additives is likely to be less than the effect on the solvents themselves. In the event that the effect of contaminants proves to be significant, the team will move to the next best class of additives.
Inability to synthesis amphiphilic molecules containing the desired moieties.	Moderate	Low	While the amphiphilic molecules are most desired, other forms of the additives will likely also be effective.

Risk Management – Cont.

Resource Risks			
Inability to locate qualified staff.	Moderate	Low	The key personnel are all leaders in their fields with strong networks of academic and industrial collaborators who can provide employment referrals. In the event that adequate staff are not located and in place for the start of the project, the key personnel will serve in their roles temporarily to avoid delays while the staff members are put in place.
Loss of senior team member.	Low	High	The loss of any key team members during the process is not expected. All the key personnel are highly committed to the organizations and to the success of the project. However, the staff members that will be added for the project will be trained by the key personnel in the early stages, so that they could continue to execute the project under the supervision of the PI in the event of a key loss.
Lack of availability of necessary analytical resources.	Low	Low	LIS has access to nearly all the equipment necessary at its facility. Where exceptions exist the pieces of equipment have been included in the budget for the project. In the unlikely event that a key gap is discovered, Dr. Zhou will attempt to locate an alternate facility through her contacts at the University of Pittsburgh, Carnegie Mellon University, and the numerous commercial laboratories in the Pittsburgh area.

Liquid Ion Solutions

Risk Management – Cont.

Management Risks			
Project estimates are inadequate.	Moderate	Low	As PI, Dr. Zhou is supported by two experienced PIs, Drs. Luebke and Nulwala, within LIS. She has been assisted in the development of the cost estimates by those managers as well as the experienced co-PIs at CMU and CCS. In the event that estimates are inaccurate, she will work closely with her project manager to revise the scope as necessary to ensure the goals of the project are still met.
Collaboration problems among the organizations	Low	High	In addition to being seasoned professionals with considerable experience in their fields, the project team has worked with the PI and one another in the past and all have good working relationships. It is unlikely that any significant complications will arise, but if they do, the PI will work to resolve them quickly to prevent any impact to the project schedule.
IP Risks			
IP agreements not reached with sub-contractors	Low	Moderate	The necessary agreement has already been signed with Carbon Capture Scientific and CMU.
Patents will be required for additives.	High	Low	In the event that intellectual property is developed, LIS will make use of its expertise and professional support to prosecute those patents efficiently. Drs. Luebke and Nulwala both have extensive experience in developing patent applications, and good contacts at multiple patent law firms.

Liquid Ion Solutions

Milestones: BP1

- Update Project Management Plan – 10/30/2018
- Kickoff meeting – 01/31/2019
- Complete ab initio calculations of carbamate anions and molecular dynamics (MD) simulations of hydrogen-bonded clusters/networks and viscosity for non-aqueous amine solvent systems containing carbamate anions – 06/30/2019
- Complete proof-of-concept testing with the five model additives identify at least one model compound which decreases CO_2 viscosity by 20% upon loading. The loading of the additive should not be more than 10 wt% of the solution – 09/30/2019
- Develop quantitative correlation between viscosity of the solvent and the equipment types and operation costs in solvent-based carbon capture process – 09/30/2019

Liquid Ion Solutions

Success Criteria: BP1

- Successful completion of all work proposed in Budget Period 1
- For two of the three selected model solvents, a reduction of 20% in solvent viscosity upon addition of less than 10 wt% additive and with less than 10% loss in CO_2 capture capacity in comparison with the corresponding neat solvents
- Preliminary Engineering Analysis to demonstrate that potential solvent with additive will save capital cost by 5%

Liquid Ion Solutions

Milestones: BP2

- Complete screening of ether and ester additives by MD analysis of their efficiency in disrupting hydrogen-bond network and reducing viscosity of the CO_2 solvent system. Recommend three additives based on these computational model calculations – 03/31/2020
- Complete synthesis and evaluation of the three additives suggested by the computational model – 09/30/2020
- Establish preliminary correlation between the cost of potential additives to be used in the solvent and the savings in equipment and operation costs in solvent based carbon capture processes – 09/30/2020

Liquid Ion Solutions

Success Criteria: BP2

- Successful completion of all work proposed in Budget Period 2
- Achieve at least 50% solvent viscosity reduction with addition of less than 10 wt% additive and less than 10% loss in CO_2 capture capacity
- Preliminary Cost Benefit Analysis shows that the successful solvent with additive could reduce the cost of CO_2 capture by at least $1/tonne

Liquid Ion Solutions

Milestones: BP3

- Complete synthetic flue gas testing for optimized additive-solvent system showing that the additives would decrease the viscosity by 50% of the model compounds with additive concentration less than 5 wt% – 03/31/2021
- Finalize the cost benefit analysis and provide future guidance for the similar projects – 09/30/2021

Liquid Ion Solutions

Success Criteria: BP3

- Successful completion of all work proposed
- Completion of lab-scale testing, including 100 absorption/regeneration cycles with simulated flue gas; lab-scale testing results showing a 50% viscosity reduction with additive concentration less than 5% and less than 5% loss in CO_2 capture capacity
- Submission of an updated: (1) State-Point Data Table and (2) Cost Benefit Analysis. Final cost benefit analysis shows a reduction in CO_2 capture cost of at least $2/tonne
- Submission of a Final Report

Liquid Ion Solutions

Schedule – BP1

Liquid Ion Solutions

Schedule – BP2 and BP3

		Year 1				Year 2				Year 3			
	Cost	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 5.0 – Computational Additive Screening	$222,316												
Task 5.1 – Computational Design of Hydrogen Bonding Disruptors								MF5					
Task 5.2 – Simulation of the Effect of Additives on Viscosity													
Task 5.3 – Incorporation of Experimental Results													
Task 6.0 – Additive Screening and Optimization	$395,060									MG6			
Task 6.1 – Additive Structure Optimization and Synthesis										DP2			
Task 6.2 – Additive Loading Optimization Study													
Task 7.0 – Preliminary Cost Benefit Analysis	$47,480												
Task 7.1 – Experimental Data Review and Cost Estimation									MH7				
Task 7.2 – Preliminary Cost Benefit Analysis with Selected Additives													
Task 8.0 – Synthetic Flue Gas Study	$445,832												
Task 8.1 – Synthetic Flue Gas Testing													
Task 8.2 – Cycle Testing for Evaluation of Degradation Products											MI8		
Task 9.0 – Develop Cost Benefit Model	$80,824												
Task 9.1 – Cost Benefit Analysis Revision													M9J
Task 9.2 – Additive Sensitivity Analysis													

DP3

M = Milestone

DP = Decision Point

Liquid Ion Solutions

Budget

	Budget Period 1 10/01/18-09/30/19		Budget Period 2 10/01/19-09/30/20		Budget Period 3 10/01/20-09/30/21		Total Project	
	Government Share	Cost Share	Government Share	Cost Share	Government Share	Cost Share	Government Share	Cost Share
LIS	$577,511	$143,529	$425,020	$105,323	$435,862	$108,966	$1,438,393	$357,817
CCS	$74,011	$18,503	$27,872	$6,968	$47,445	$11,861	$149,328	$37,332
CMU	$126,209	$32,401	$129,760	$33,372			$255,969	$65,773
Total	$777,731	$194,433	$582,652	$145,663	$483,307	$120,827	$1,843,690	$460,922
Cost Share	80%	20%	80%	20%	80%	20%	80%	20%

Liquid Ion Solutions

Initial Results

Liquid Ion Solutions

Progress in Computational Study of CO_2 Solvents

Objectives and accomplishments during 8/1/18-9/30/18:

1. Constructed a reliable force field model based on OPLS-AA and ab initio calculations. Test simulations using the force-field model we constructed show good agreement with experiments in density and viscosity.
2. Tested different methods for viscosity calculations. It was found that the nonequilibrium periodic perturbation method is most robust.
3. Systems we studied thus far include 2-methoxyethylamine and 2-(methylamino)ethanol.

Liquid Ion Solutions

MD Results for Solvent Density

T = 300 K
Units: g/mL

Solvent	Simulated density	Experimental value
2-methoxyethylamine	0.865	0.864
2-(methylamino)ethanol	0.945	0.936
bis(2-methoxyethyl)amine	0.918	0.902

Very good agreement with experimental results (error < 2%)!

Liquid Ion Solutions

MD Results for Viscosity

Method: periodic perturbation method (PPM)
T = 300 K
Units: cP

Molecule	Simulated viscosity	Experimental value
2-methoxyethylamine	0.59	0.66
2-(methylamino)ethanol	11.51	10.51
bis(2-methoxyethyl)amine	-	-

1. Good agreement with experimental results.
2. PPM method was found to work better than Green-Kubo method.

Liquid Ion Solutions

Plan for BP1

Objective: Obtain theoretical understanding of (1) the relationship between hydrogen-bonded structure and viscosity of and (2) the effect of hydrogen-bond disruptors on viscosity

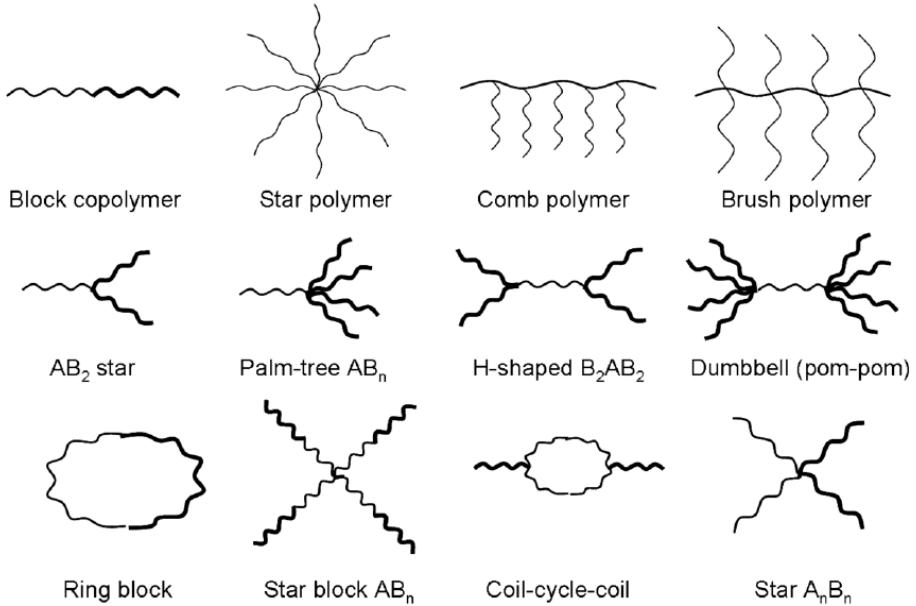
Action items:

1. Complete simulations of bis(2-methoxyethyl)amine.
2. Construct force field for the ammonium cations and carbamate anions based on OPLS-AA with the aid of ab initio calculations.
3. Study hydrogen bonded structure and viscosity of CO_2 loaded solvents, i.e., carbamate systems, via MD using the results of #2.
4. Investigate the effect hydrogen-bond acceptors, e.g., DMSO, on hydrogen-bonding network/clusters and viscosity using MD.

Liquid Ion Solutions

Initial Progress (LIS)

- In negotiation for acquiring testing equipment
- Several HB acceptors designed



Some common polymeric architectures used as viscosity modifiers

Liquid Ion Solutions

Acknowledgement and Disclaimer

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

Liquid Ion Solutions