# Universal Solvent Viscosity Reduction via Hydrogen Bonding Disruptors

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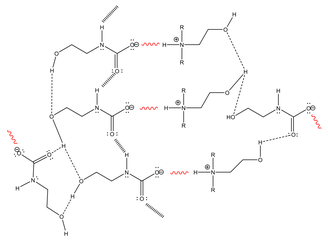
## INTRODUCTION

The goal of the project will be to achieve lab-scale demonstration of an additive system capable of decreasing the viscosity of selected non-aqueous chemical solvents for post-combustion capture of carbon dioxide. The project will build on work previously conducted by researchers at Liquid Ion Solutions (LIS), Carnegie Mellon University (CMU), and Carbon Capture Scientific (CCS), utilizing their knowledge of materials development, computational predictions of material properties, and engineering analysis of power systems, respectively.

### The problem



Hydrogen bonding networks in capture solvents result in an increase of viscosity.

**Aqueous amine drawbacks:**

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

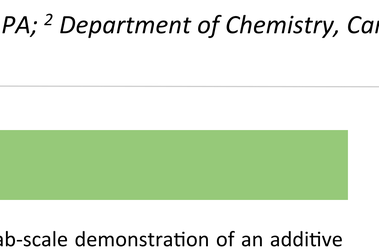
**Non-aqueous amine drawbacks:**

- High viscosity.

## OUR APPROACH

### Hydrogen bonding segmentation

The aim is to break down the overall size of the hydrogen bonding network by introducing additives which disrupt the overall network forming smaller segmented networks.




Additive effect on Viscosity (*J. Chem. Thermodyn*. **2017**, 113, 358.)

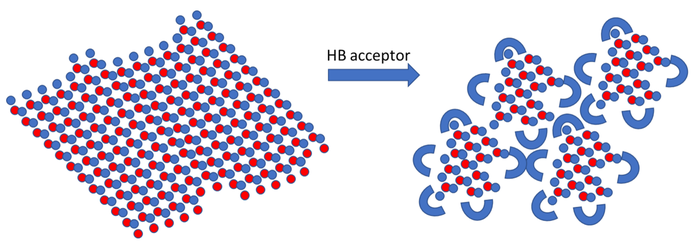
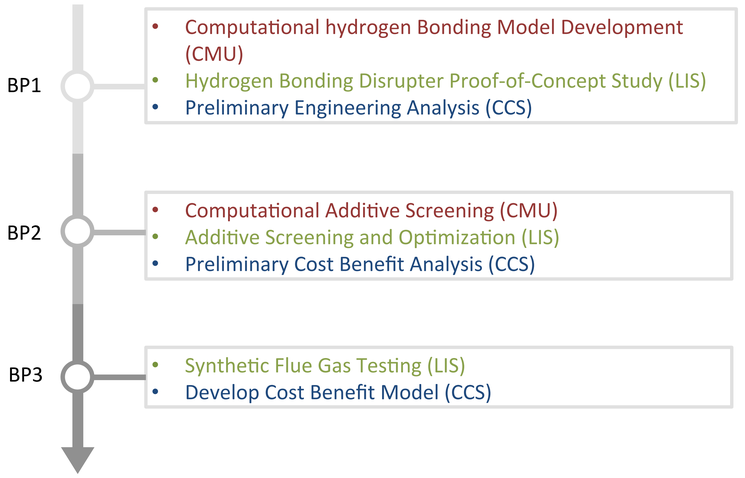



Illustration of a fully hydrogen bonded network (left) and the breakage of the hydrogen bonding network by addition of hydrogen bond acceptors (right).

## PROJECT TIMELINE

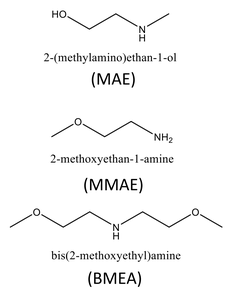



## COMPUTATIONAL STUDY

### Viscosity and hydrogen-bond network

Detailed analysis of (i) viscosity and (ii) size distribution of hydrogen-bonded clusters of three amine solvents, MMAE, MAE and BMEA, as a function of ammonium/carbamate ion concentration:

- *Ab-initio* calculations to determine force field parameters, in particular, partial charges of ammonium and carbamate ions.
- Molecular Dynamics (MD) simulations to study (i) viscosity, (ii) hydrogen-bonded structures and (iii) kinetics of hydrogen-bond formation and breaking.




Chemical structure of the amines chosen as models for the study

### Effects of hydrogen-bond disruptors

Quantitative study of the effects of hydrogen-bond disrupting additives using *ab-initio* and MD methods:

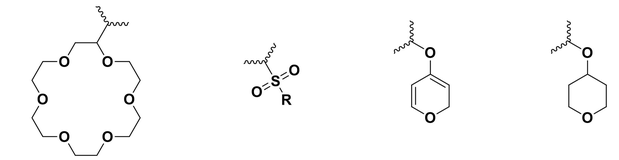
- How do they influence 3-dimensional hydrogen-bond structures of the absorbents as well as their hydrogen-bonded cluster lifetime?
- How do they modulate viscosity?
- What are the key factors that govern the disruption of hydrogen-bond structures?

As candidates for effective disruptors, we will consider oxy-dibenzene, pyran, crown-ethers, and dimethyl sulfoxide like moieties.

## HB DISRUPTER SYNTHESIS AND TESTING

### Proof-of-concept study

- Candidate selection based on computational study.
- Viscosity testing at uncharged, $CO_2$-charged, and after desorption states.



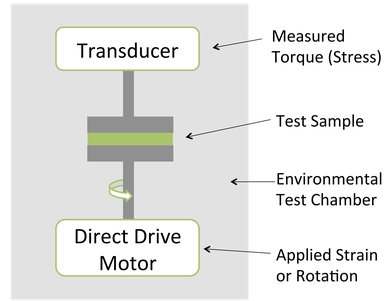

Proposed molecular functionalities for hydrogen bonding disruptors.

### Additive screening and optimization

- Additive concentration optimization.
- Evaluation of working capacity and viscosity.

### Synthetic flue gas testing

- Evaluation of optimized additive/ solvent in synthetic flue gas.
- Evaluation of working capacity and viscosity after multiple cycles.




Model solvents will be evaluated using a rheology testing system in an environmental test chamber.

## ENGINEERING ANALYSIS

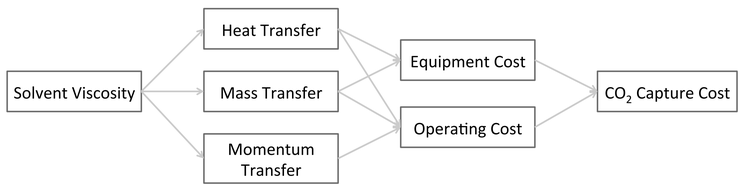
### Preliminary engineering analysis

Examining the impacts of viscosity on momentum, heat and mass transfer in carbon capture systems.

### Preliminary cost benefit analysis

Use of additives to reduce solvent viscosity in post-combustion capture processes.

### Development of cost benefit model




## ACKNOWLEDGEMENT

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