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 (UIS), 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

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 networks in capture solvents result in an increase of viscosity.

Project Timeline

- Computational hydrogen Bonding Model Development (CMU)
- Hydrogen Bonding Disruptor Proof-of-Concept Study (UIS)
- Preliminary Engineering Analysis (CCS)

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.

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, CO₂-charged, and after desorption states.

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.

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

Liquid Ion Solutions, Carnegie Mellon University, and Carbon Capture Scientific gratefully acknowledge the support of the United States Department of Energy's National Energy Technology Laboratory under agreement DE-FF001629 for funding the work.

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