Universal Solvent Viscosity Reduction via Hydrogen Bonding Disruptors

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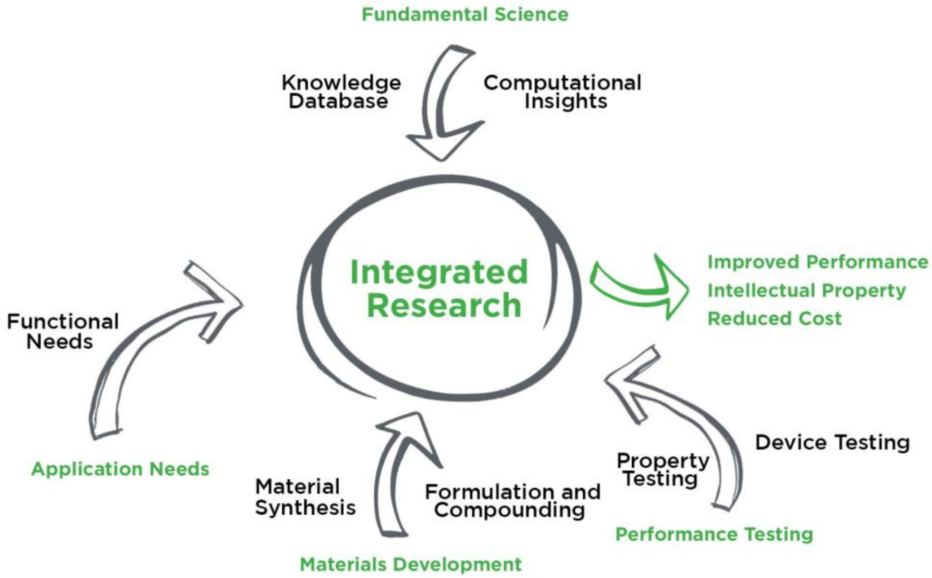
Materials Innovation at RoCo Global

ROCO

Reduce CO_2

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.



Capabilities

Synthesis

- Small scale and scale-up (up to 22L) synthesis capabilities

Processing

- Bench-scale compounder
- Twin screw extruder (w/ palletizer & film casting)
- CryoMill

Testing

- FT-IR
- GC-FID
- HPLC & GPC
- Thermal analysis (TGA & DSC)
- Rheometer
- Viscometer
- Multiparameter testing system
- Lab-scale absorption/desorption system

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

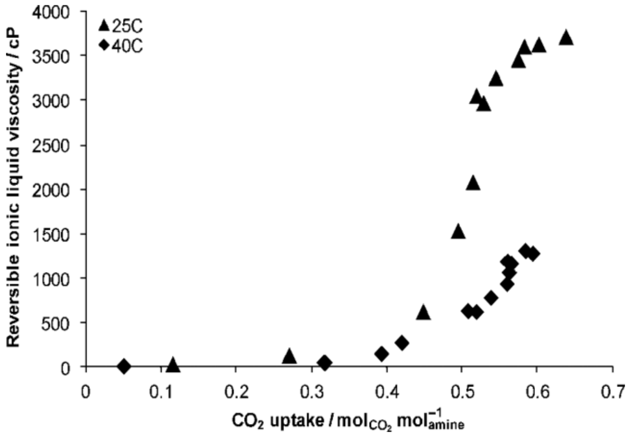
The project goal is to develop additives capable of decreasing viscosity of water-lean solvents for post-combustion capture.

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

	NETL Case 10 (MEA)	Water-lean solvents
Estimated reboiler duty (Btu/lb CO_2)	1520	753-1100
Net plant efficiency (HHV)	25.4%	27.5-32.5%
Cost per tonne CO_2 capture (USD)	60	39-63



Viscosity as a function of CO_2 loading for a water-lean silylamine.

Solvent viscosity coupled with CO_2 capture capacity has a major impact on overall capture cost

Chem. Rev. **2017**, *117, 9594-9624; DOE/NETL-2010/1397*; 2011; *ChemSusChem* **2010**, *3* (8), 919–930; *Energy Fuels* 2012, 26, 4, 2512–2517; *Energy Procedia* **2014**, *63*, 580–594; Energy Procedia, 2013, 37, 285-291; *Energy Environ. Sci.* **2013**, *6* (7), 2233 *Energy Environ. Sci.* **2020**, *13* (11), 4106–4113; *ChemSusChem*, **2014**, 7: 299-307

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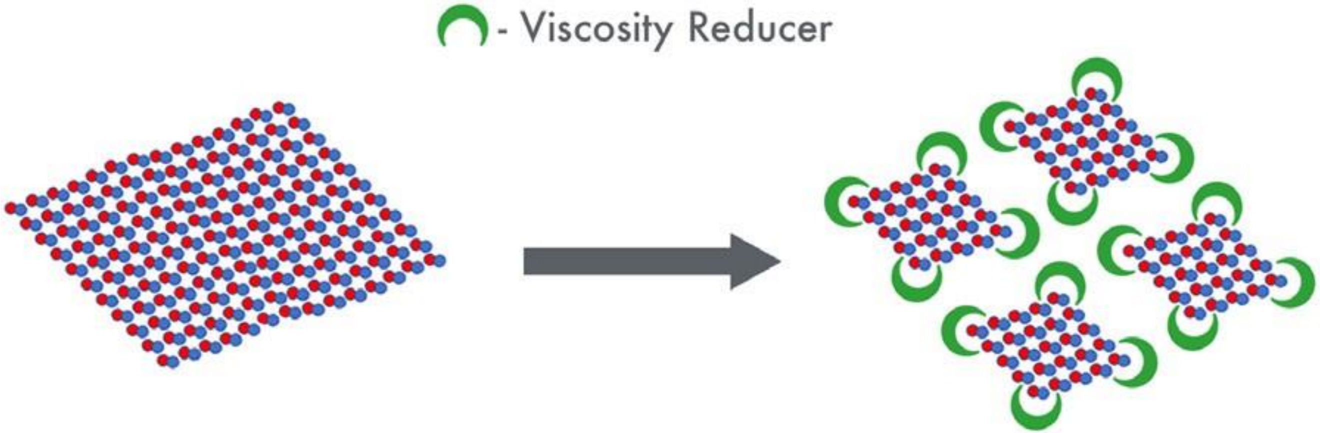
RoCo's Additive Approach to Reduce Viscosity



Hydrogen bonded network

High viscosity

Segmentation of hydrogen bonded network

Low 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.

Project Scope and Schedule

Budget Period 1	Budget Period 2	Budget Period 3
10/1/2018-9/30/2019	10/1/2019-9/30/2020	10/1/2020-9/30/2021
Computational hydrogen Bonding Model Development	Computational Additive Screening	
Hydrogen Bonding Disrupter Proof-of-Concept Study	Additive Screening and Optimization	Synthetic Flue Gas Testing
Preliminary Engineering Analysis	Preliminary Cost Benefit Analysis	Develop Cost Benefit Model

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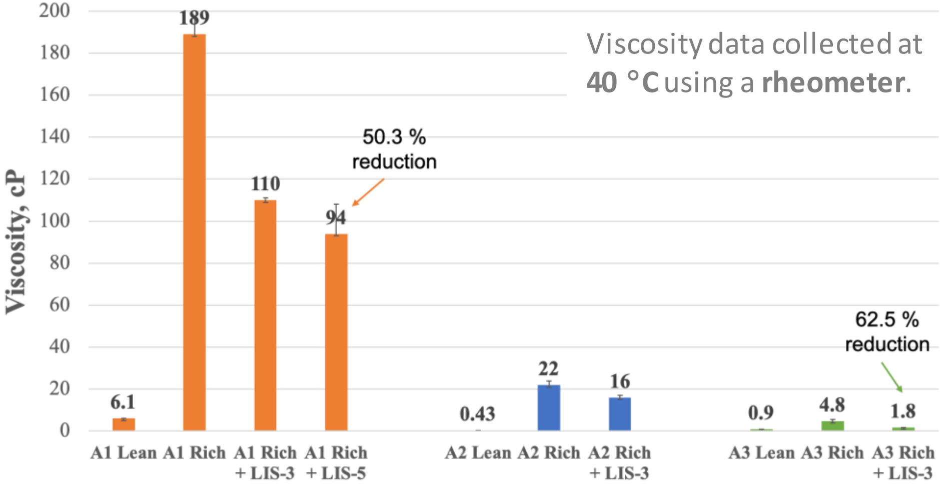
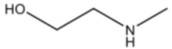
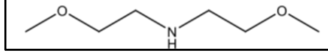
BP1 Accomplishments

- 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.



Model solvents

Chemical structure	Abbr.
	A1
	A2
	A3

A1 and A2 rich samples contained ca. 18 wt% CO_2, A3 rich samples contained 9 wt% CO_2.

- 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.

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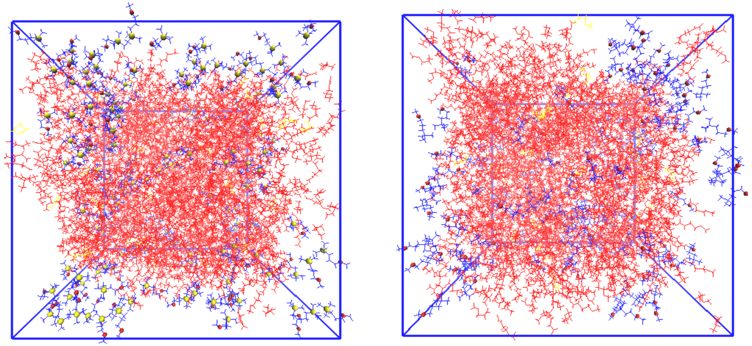
BP2 – Computational Additive Screening

- 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.



MTS: 118 cP MDP: 259 cP

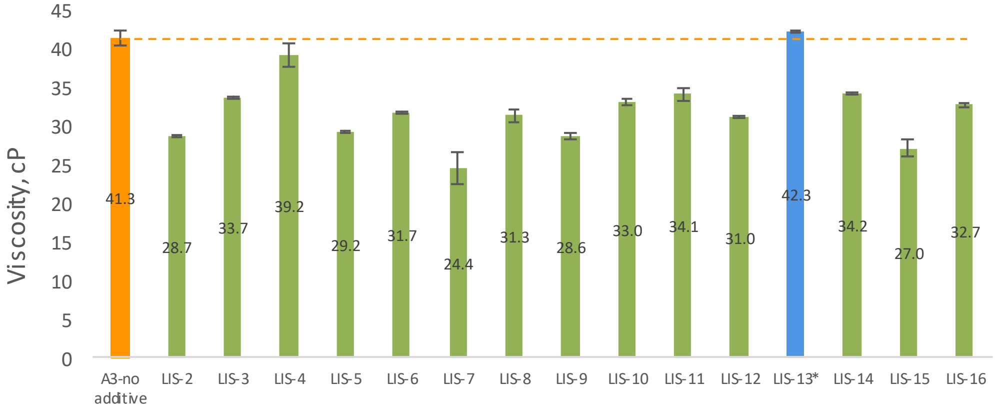
Additives mainly locate at interfacial region between hydrogen-bonded cluster and bulk A2

Insights gained from simulation study

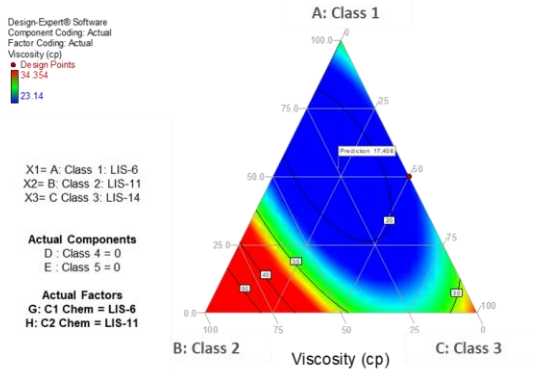
- Important factors: large van der Waals volume; good flexibility; week hydrogen-bond accepting power.
- Recommended 3 specific additives for experiment.

BP2 – Experimental Additives Development

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



5% additive loading in A3; data collected at r.t. using a viscometer



RoCo developed proprietary viscosity-reducing additives that can reduce viscosities of model amine solvents up to 50% upon CO_2 loading.

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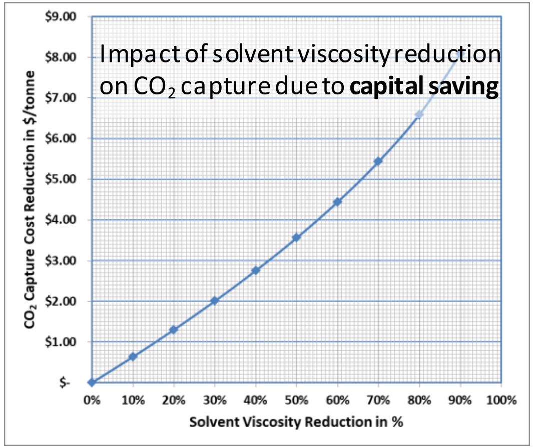
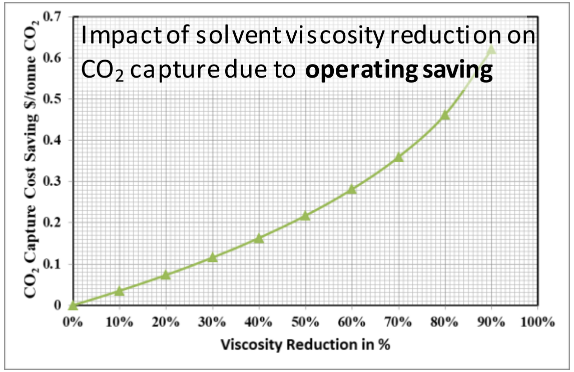
BP2 – Preliminary Cost Benefit Analysis

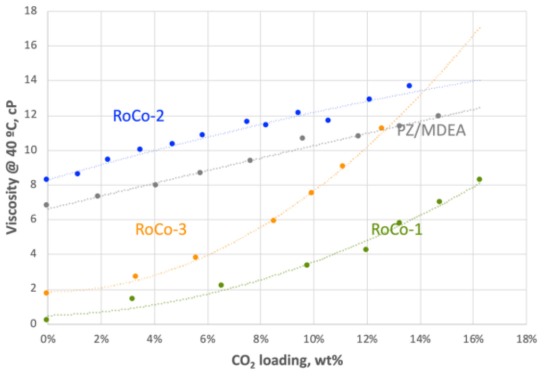
- Net benefit generated from adding viscosity-reducing agent (additive) into the solvent is significant.
- Additive approach significantly exceeds the targeted success criteria of \$1/tonne CO_2 captured.
- The cost of additive compared to the benefit is insignificant.
- Based on this analysis, the cost 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.

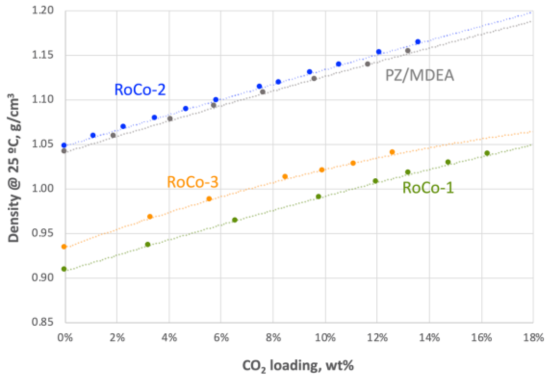


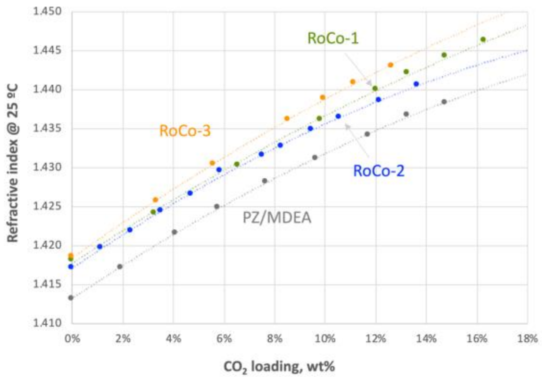


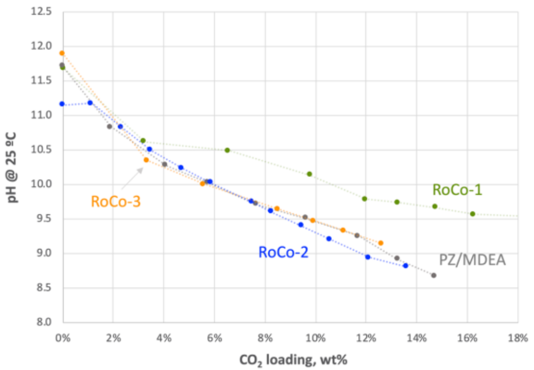
BP3 – Synthetic Flue Gas Study

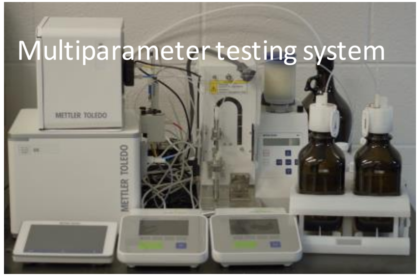
Testing methods development and baseline testing











BP3 – Synthetic Flue Gas Study – cont'd

RoCo lab-scale testing unit

Process conditions

Parameter	Value
Gas flow rate	Various: 1-11 ±0.1 SLPM
CO_2 in gas composition	4±0.5; or 15±0.5 vol%
Solvent flow rate	Various: 5-30±1 mL/min
Absorber temperature	40±5 °C
Stripper temperature	Various: 90-120±5 °C

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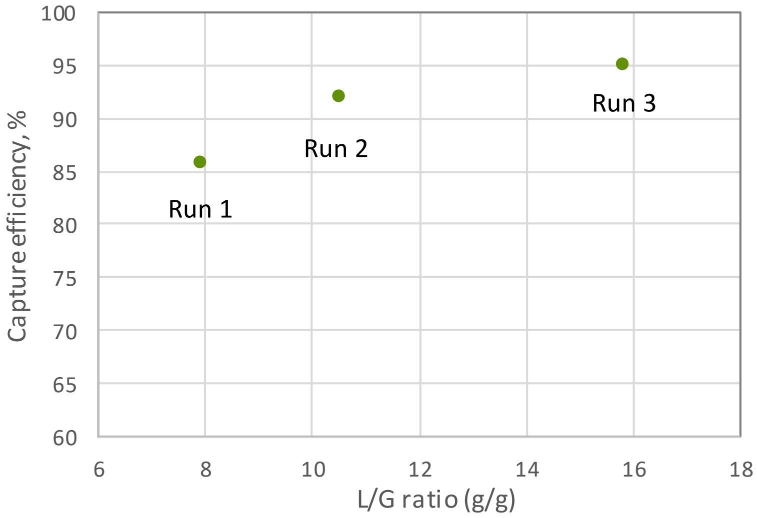
BP3 – Synthetic Flue Gas Study – cont'd

Absorption tests



Run #	Solvent type	CO_2 uptake (wt%)	Viscosity @ 40 °C (cP)	Density (g/cm^3)	Refractive index	pH
1	Lean	0.22 ±0.15	1.323 ±0.004	0.92794	1.4204	10.78
	Rich	4.82 ±0.27	2.987 ±0.015	0.97758	1.4307	10.00
2	Lean	0.14 ±0.02	1.225 ±0.006	0.92350	1.4199	10.95
	Rich	4.41 ±0.46	2.288 ±0.626	0.97010	1.4295	10.06
3	Lean	0.13 ±0.03	1.622 ±0.009	0.93703	1.4197	10.90
	Rich	4.75 ±0.32	3.337 ±0.027	0.98411	1.4296	10.07

Absorption runs of an amine-additive solvent achieved up to 95% capture efficiency under simulated flue gas containing 15 vol% CO_2. We observed a viscosity of less than 5 cP with CO_2 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_2 loading.
- Absorption runs of an amine-additive solvent achieved up to 95% capture efficiency under simulated flue gas containing 15 vol% CO_2. We observed a viscosity of less than 5 cP with CO_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_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_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

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

- DOE Program Manager: Katharina Daniels and Andrew Jones
- Project partners:

Carnegie Mellon University

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Thank you!

Any Questions?

Appendix

Organization Chart

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

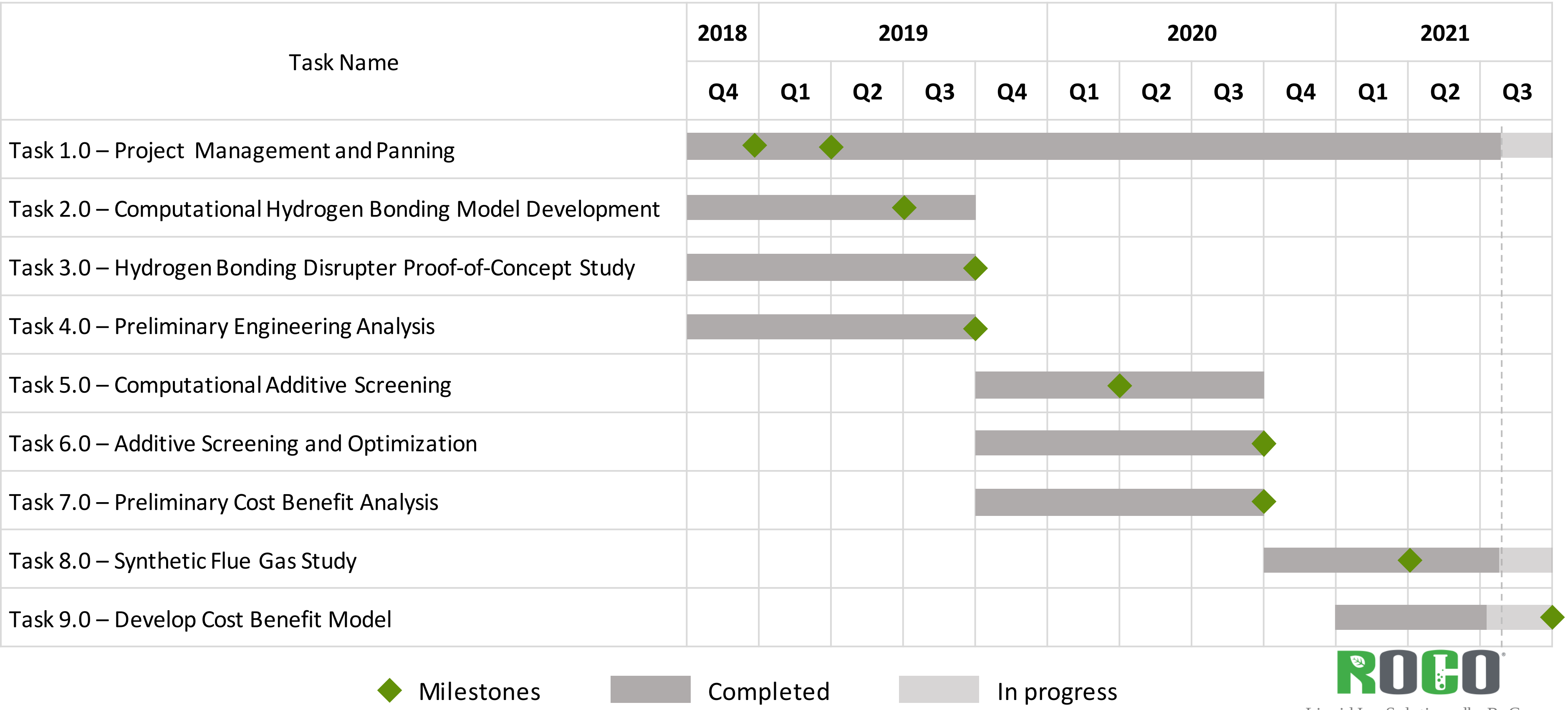
Carnegie Mellon University

- 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


Task Name
2018
2019
2020
2021
Q4
Q1
Q2
Q3
Q4
Q1
Q2
Q3
Q4
Q1
Q2
Q3
Task 1.0 – Project Management and Panning
Task 2.0 – Computational Hydrogen Bonding Model Development
Task 3.0 – Hydrogen Bonding Disrupter Proof-of-Concept Study
Task 4.0 – Preliminary Engineering Analysis
Task 5.0 – Computational Additive Screening
Task 6.0 – Additive Screening and Optimization
Task 7.0 – Preliminary Cost Benefit Analysis
Task 8.0 – Synthetic Flue Gas Study
Task 9.0 – Develop Cost Benefit Model
Milestones
Completed
In progress