### Demonstration and Validation of Additively Manufactured Intensified Device for Enhanced Carbon Capture

Project Number: FEAA375

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> U.S. Department of Energy National Energy Technology Laboratory **Carbon Capture 2020 Integrated Review Webinar** October-5-7 2020

# **Program Overview**

- Funding provided by DOE-FE: \$500k
- Overall Project Performance Dates:
  January 1, 2020 December 31, 2020
- Project Participants:

Costas Tsouris, Canhai Lai, Eduardo Miramontes, Lonnie Love, Gyoung Jang, Xin Sun

# **Overall Project Objectives**

- Demonstrate enhanced CO<sub>2</sub> capture using ORNL's intensified packing device with low aqueous solvent
- Simulate process with the objective to design a bigger column for enhanced CO<sub>2</sub> capture with intensified packing devices

## **Technology Background**

How the technology is envisioned to work in operation:



Absorption/Desorption System at the National Carbon Capture Center NCCC)  $2MEA + CO_2 \rightleftharpoons MEAH^+ + MEACOO^- (+ 79-100 \text{ KJ/mol}) \text{ (Exothermic)}$ Intensified packing device to allow *in situ* cooling 4

### **Technology Background** Technology development efforts prior to current project:





**Question**: How can we manufacture a device like this to also work as a heat exchanger?

• System tested for hydraulic and heat transfer performance with favorable results Miramontes, E.; Love, L.J.; Lai, C.; Sun, X.; Tsouris, C. Additively Manufactured Packed Bed Device..., *Chem. Eng. J.*, **388**, 124092, (2020). <sup>5</sup>

### **Technology Background** How the technology was tested for CO<sub>2</sub> capture:





Schematic of testing facility and absorption column CPE: Commercial Packing Element

# **Technology Background**

Advantages of the technology:

Air Flow Rate (LPM)	CO <sub>2</sub> Flow Rate (LPM)	CO₂ Conc. (%)	Molar Capture Rate Before Cooling (mol/min)	Molar Capture Rate After Cooling (mol/min)	Fractional Increase (%)	Capture Efficiency(%) (Before → After Cooling)
810	90	10	2.24	2.30	2.7	59.9 → 61.2
510	90	15	2.75	2.90	5.5	73 → 77
360	90	20	2.95	3.29	11.5	78 → 88
264	90	25	3.52	3.57	4.3	94 → 98
360	40	10	1.38	1.45	5.1	83 → 87
360	63.5	15	1.53	1.77	15.7	58 → 67
360	90	20	2.95	3.29	11.5	78 → 88
360	120	25	3.07	3.28	6.9	62 → 66

Solvent flowrate: 3.2 LPM

Solvent input temperature: 70 °C

 Miramontes, E.; Jiang, E.A.; Love, L.J.; Lai, C.; Sun, X.; Tsouris, C. Process Intensification of CO<sub>2</sub> Absorption Using a 3D Printed Intensified Packing Device, *AIChE J.* e16285, (2020).

# **Technology Background**

#### Technical and economic comparisons:

	HEX-Packing Device	Commercial Mass-
	(Intensified Packing Device)	Transfer Devices
Multifunctionality	Yes	No
Maximum surface area utilization	Yes	No
Design flexibility	Yes	No
Process footprint	Low	High
Process complexity	Low (eliminates the need of	High
	external heat exchangers)	
Price	Less than \$5,000	Less than \$5,000
Pressure drop	Can be controlled by adjusting	Lower
	density of corrugated plates	
Flooding	Can be controlled by adjusting	At higher flow rates
	density of corrugated plates	
Controllability of surface	High	High
functionality (hydrophobicity/		
hydrophilicity, surface roughness)		
Intrinsic Thermal Exchange	Yes	No

### Technology Background Modeling:

- MFIX Solvent Model
  - A CFD module developed in NETL's Multiphase Flow with Interphase eXchanges (MFIX) software suite that incorporates basic property data and basic data sub-models to capture the behavior of CO<sub>2</sub> absorbing MEA using the two-fluid model (TFM) and discrete element model (DEM) approaches
  - Validated previously by experimental data
- CFD simulations applying MFIX Solvent Model
  - Plan simulations to sweep through the realistic design space, i.e., position of the intensified device and desired cooling capability, to identity the optimal location of the intensified device for different operating conditions
  - A design of experiment will be established for the subsequent experimental validation
  - Results from the CFD device-scale model can then be used to inform system scale optimization

# Technical Approach/Project Scope

Motivation for the current project:

- The intensified device was used to enhance CO<sub>2</sub> capture by MEA
- Aqueous amines, however, such as MEA, have drawbacks including volatility and high regeneration energy
- Low/non-aqueous solvents could reduce energy cost and solvent loss
- Energy of regeneration has three components:

$$q_R = \left[\frac{c_p(T_R - T_F)}{\Delta \alpha} \cdot \frac{M_{sol}}{M_{CO_2}} \cdot \frac{1}{x_{sol}}\right] + \left[\Delta H_{V,H_2O} \cdot \frac{p_{H_2O}}{p_{CO_2}} \cdot \frac{1}{M_{CO_2}}\right] + \left[\frac{\Delta H_{abs,CO_2}}{M_{CO_2}}\right]$$
  
Sensible Heat Vaporization Heat Absorption Heat

- Low-aqueous solvents have lower specific heat than water, reducing sensible heat but also increasing temperature swing
- Intercooling is thus expected to have a more significant impact on CO<sub>2</sub> capture than in aqueous solvents
- Applicability of intensified device to low aqueous systems is being investigated in the current project

#### Technical Approach/Project Scope Experimental design and work plan:

- Testing of the intensified device with MEA solution required heating the solvent to 70 °C due to the relatively low flowrates
- The heat capacity of low-aqueous solvent, however, is approximately half of the heat capacity of the MEA solvent
- Because of its lower heat capacity, the low-aqueous solvent is expected to heat up faster due to the exothermic reaction
- Thus, for testing with low-aqueous solvent, we plan to warm up the input solvent at lower temperatures than the 70 °C used for MEA.
- A 30-gallon tank of low-aqueous solvent was provided by RTI, thanks to Marty Lail and his team, for this project
- This solvent was not fully compatible with column materials 11

#### Technical Approach/Project Scope Experimental system modifications:



### Technical Approach/Project Scope Project schedule:

- This one-year project has the following tasks:
  - 1. Project management
  - 2. Column-scale demonstration of enhanced capture
    - 2.1. Reconstruction of Column A for low-aqueous solvent capture
    - 2.2. Quantification of capture efficiency with commercial packing
    - 3.3. Quantification of capture efficiency with intensified packing
  - 3. Column-scale computation scoping for the conceptual design
    - 3.1. Calibration of ORNL MFiX model with results from Column A
    - 3.2. Computational scoping for flexible, modular, enhanced capture

<u>Note:</u> Column A is the column we used for the MEA solvent Column B will be designed and constructed for future work

# Technical Approach/Project Scope

Project success criteria, risks, and mitigation strategies:

#### Project success criteria:

- 1. Experimentally prove enhanced CO<sub>2</sub> capture efficiency with intensified device compared to MellaPak baseline, for low-aqueous solvent
- 2. Computationally obtain conceptual design and associated operating conditions for Column B which demonstrate greater than 10% capture efficiency for MEA with intensified device

#### Project risks and mitigation strategies:

- 1. Addition of a new solvent introduces potential new safety hazards Mitigation strategies were outlined by ORNL safety personnel
- Lack of accurate models and experimental data introduce uncertainty in predictive results of capture efficiency and operating conditions Computational modeling will be combined with process modeling and empirical design
- 3. Covid-19 related facility shut down leading to delays

# Technical Approach/Project Scope

Identify optimal conditions through the realistic design space:

- Apply previously validated (Column A) MFIX Solvent Model to perform simulations within realistic design space to find optimal operation conditions for Column B
  - Column height
  - Solvent and gas flows
    - $\circ~$  Flow rates, species concentration, inlet temperature
  - Intercooling
    - o Locations, temperature
- Compare with simulation results using Aspen+ based process model (collaborating with West Virginia Univ.)

# Progress and Current Status of Project

Description of the test equipment used/built in the project:



- The PVC tube was replaced by a polyethylene tube
- New pump was added for the delivery of low-aqueous solvent
- Thermocouples were placed between
  consecutive packing elements to monitor the temperature profile

Reconstructed column (top) and thermocouple placement (right)

T<sub>1.9</sub> (18.7 in)

acki

T<sub>1,8</sub> (37.75 in)

#### **Progress and Current Status of Project** Hydraulic testing of the modified equipment:



Measurement error: ~6% (N=3)

Liquid holdup and pressure drop behaved as expected <sub>17</sub>

# **Progress and Current Status of Project**

Identify Optimal Conditions through Realistic Design Space:



Gas

## **Progress and Current Status of Project**

Inlet temperature and cooling effect:

- Cooling effect on CO<sub>2</sub> capture depends on inlet temperature
  - 90 °C: capture improves from 53.8% to 81.6%
  - 70 °C: capture improves from 68.4% to 82.6%
  - 50 °C: capture improves from 76.9% to 81.7%
  - 40 °C or lower: cooling hurts CO<sub>2</sub> capture

#### Conclusion

- Cooling effectiveness on improving CO<sub>2</sub> capture is more obvious when inlet temperature is higher
- Implication: less cooling needed before entering absorber column



#### **Progress and Current Status of Project** Effect of Cooling Section Configuration:

- Distributed cooling sections improve CO<sub>2</sub> capture
  - 90 °C: CO<sub>2</sub> capture efficiency:  $53.8\% \rightarrow 76.9\% \rightarrow 81.6\%$
  - 70 °C: CO<sub>2</sub> capture efficiency:  $68.4\% \rightarrow 77.8\% \rightarrow 82.6\%$



#### **Progress and Current Status of Project** Significant accomplishments and how they tie to the technology challenges:

- Obtained low aqueous solvent from RTI International and prepared experimental protocols to safely perform experiments
- Modified experimental setup with materials compatible with the low-aqueous solvent
- Performed hydraulic testing to make sure that the equipment performs as expected
- CO<sub>2</sub> capture experiments using low-aqueous solvent are expected to start in the first week of October
- Computational modeling shows that the cooling effect on CO<sub>2</sub> capture depends on the inlet temperature of the solvent

#### **Progress and Current Status of Project** Performance levels achieved in experiments so far:

- There is a delay in the performance due to Covid-19
- According to the original schedule, experiments without cooling by the intensified packing device should have been completed by now
- The delay will be eliminated in the last quarter of the project (October 1 December 31)
- The protocol for the experiments has two parts:
  - Run the CO<sub>2</sub> capture experiment without cooling until steady state is achieved
  - After steady state is achieved, start cooling by introducing cold water through the intensified device

In this way, the same-quality solvent will be used for a better comparison between cooling and non-cooling conditions

## Plans for Future Testing/Development/ Commercialization

- A patent application describing the manufacturing of the intensified packing device has been submitted to the U.S. Patent Office, and is currently pending
- The technology is ready for commercialization
- This project brought together a collaboration between ORNL and RTI International that is expected to help the commercialization of the intensified device
- R&D 100 Award Finalist status and a press release in June 2020 also help the publicity of the invention
- A new project with multiple CRADA partners, funded by the DOE Technology Commercialization Fund (Topic 1), is about to start with the objective to improve the device toward commercialization

## Plans for Future Testing/Development/ Commercialization

- The intensified device can be scaled up to  $\sim 20$  inches diameter
- Scale-up will be pursued with Column B in a follow-up project



# Summary Slide

- The current project is expected to be completed in time, on December 31, 2020
- Work in all tasks has progressed well
- A slight delay in the experimental program due to Covid-19 is expected to be eliminated in the remaining quarter
- Intellectual property has been secured
- Efforts toward commercialization are progressing well
- Modeling work is on schedule

Thanks to all the contributors, Program Manager, and the Sponsor of the project

# Appendix

### Organization Chart FEAA375

- Task 1. Project Management (Xin Sun and Costas Tsouris; ORNL)
- Task 2. Column-scale demonstration of enhanced capture
  - Solvent (Marty Lail and Paul Mobley; RTI) (no cost to this project)
  - Intensified packing device (Lonnie Love; ORNL)
  - Experimental setup (Costas Tsouris, Scott Palko, Eduardo Miramontes, Gyoung Jang; ORNL)
  - Experiments (Costas Tsouris and Gyoung Jang; ORNL)
- Task 3. Column-scale computation scoping for the conceptual design
  - Computational modeling (Canhai Lai; ORNL)
  - Process modeling (Ryan Hughes and Debangsu Battacharyya;

West Virginia University) (no cost to this project)

### Gantt Chart

