Efficient Integrated Methanol Synthesis Using Carbon from Direct Air Capture, Contract DE-FE0032400



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Project Objective





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DOE Share = \$400,000 Cost Share = \$100,000 Total Project = \$500,000

Technical PoP = 1 year

DE-FOA-0002614 AOI-2G

- Complete a Conceptual Design Study for an integrated Direct Air Capture (DAC) and Carbon Dioxide Utilization System (DACUS) that captures and utilizes CO₂ in an integrated methanol (MeOH) synthesis process
 - Design of a DACUS is based on Verde's STG+ process CO2 to methanol process that uses green H_2 to synthesize green methanol with popative carbon emissions
 - with negative carbon emissions
- Project Objectives
 - Complete a **technoeconomic analysis (TEA)** for the integrated system
 - Complete a Life Cycle Analysis (LCA) for the system
 - Conduct a **technology gap analysis (TGA)**
 - Create a technology maturation plan (TMP)
 - Develop a Community Benefits Plan (CBP), including Quality Jobs
 Plan (QJP), Diversity, Equity, Inclusion, and Accessibility (DEIA) Plan;
 Justice40 (J40) Plan



Introduction

- New DACUS process removes CO₂ from air and converts it into "green methanol" via a thermochemical process
- The H₂ used in the methanol synthesis is generated via electrolysis of water using renewable energy
- Methanol could be used as a fuel or H₂ carrier and it is a building block chemical that can be converted into other chemicals and fuels
 - E.g., synthetic green gasoline via ExxonMobil's MTG process
- Combines two transformational technologies
 - TDA's DAC process
 - Verde's STG+ process



Verde's Clean Fuel Technology



Verde Clean Fuels is a publicly traded company in NASDAQ, specializes in converting municipal waste and biowaste to methanol or gasoline



TDA's Sorbent for DAC

- TDA has been developing a new polymer sorbent for DAC and life support applications (DE-SC-00020846, 80NSSC18C0135, N00178-18-C-8009)
 - Sorbent has very high CO₂ uptake in dilute gas streams (e.g., 400 ppm CO₂ in air; 2,500 ppm spacecraft cabin; up to 5,000 ppm in submarines)
 - The sorbent maintains its stability at high temperatures
- The sorbent can be prepared in the form of pellets, laminates, 3D printed monoliths, and as coated layers on HEX surfaces



Various forms of polymer sorbent: (a) powder (b) pellets (c) single laminate layer (d) 3D printed monolith (e) applied as a coating on HEX surfaces



Preparation of Structured Sorbent







tonk

Scale-Up is in progress in collaboration with Membrane Technology Research (DE-FE0032151)



Design of DAC System

- Modular Design with easy to install Sorbent Cartridges
- Each contactor designed to the dimensions of a 40ft shipping container to allow for ease of transportation and installation







System Design

- Design Basis:
 - 100,000 MTPY CO₂ captured
 - 72,206 MTPY MeOH produced
- CO2 Capture Efficiency 90%
- Laminate microchannel contactor design
 - 10-15 mbar pressure drop
- TSA adsorption cycle
 - Adsorption at 15-40°C
 - Regeneration at 100+°C

Preliminary Carbon Balance:

Inputs	kmol/h	mol frac C	kmol/h C
Atmospheric Air	729,009	400 ppm	288
Outputs			
Exhaust Air	728,747	40 ppm	29
Crude Methanol	461	0.56	257
Vent Gas	4	0.44	2



High Temperature Oxidative Stability



- TDA identified several formulations that can provide high temperature oxidative stability
- An aggressive test method is used to accelerate aging effects in air for 24 h at 120°C under dry conditions
- CO₂ uptake performance is tested before and after the aging test in a 5 min concentration swing cycle at 60°C

Integrated Process Summary





Design of DAC System

Process Steps

- Fan draws air across structured sorbent which captures CO₂
- Contactor is then isolated to begin the regeneration process.
- Product CO₂ is heated and recirculated to pre-heat the sorbent.
- Steam sweep under slight vacuum is used to remove the adsorbed CO₂
- CO₂ is is compressed and sent to a MeOH synthesis reactor.
- Fans and compressors operate continuously.



From



Heat Integration

 MeOH synthesis is exothermic where this heat (potentially) can be co₂ used for regenerating the DAC sorbent

H₂

- MeOH reactor effluent can be cooled by raising low pressure steam for regeneration
- Additional heat sources include the overhead streams in distillation

Heat Integration Point	Available Heat (MMBTU/hr)	% of Heat Required for Regeneration
1	13.4	25%
2	11.4	21%
3	13.0	24%
4	16.8	31%



DAC Output Requirements



- CO₂ and H₂ supplied at 900 psig at a 1:3 carbon to hydrogen ratio
- Steam generated from vent gas combustion is saturated at 75 psig • Used for MeOH distillation



Heat Integration (Steam Generation)

- After adsorption, air is present in the contactor void space and is captured during regeneration
- O₂ must be removed prior to MeOH synthesis to protect Verde's catalyst
- Using catalytic oxidation, we can remove O₂ from the CO₂ stream and raise steam to support MeOH distillation
- MeOH vent gas is burned with O₂ in CO₂ stream





Life Cycle Analysis

- UC Denver will lead the LCA work
 - Dr. Arunprakasj Karunanithi's group
- Calculate carbon footprint of the DAC system
 - Cradle to gate basis mining, shipping, construction, etc.
 - Explore design approaches to mitigate upstream impacts
- Sensitivity Analysis on critical inputs to minimize CO₂ generation and optimize CO₂ consumption
- Preliminary analysis assumptions:
 - All electricity is renewable
 - Waste heat supplied by STG+



Work Plan

- Task 1. Project Management and Planning
 - Task 1.1 Project Management Plan (PMP)
 - Task 1.2 Technology Maturation Plan (TMP)
 - Task 1.3 State Point Data Table
 - Task 1.4 Preliminary Technoeconomic Analysis (TEA)
 - Task 1.5 Preliminary Life Cycle Analysis (LCA)
 - Task 1.6 Technology Gap Analysis (TGA)
 - Task 1.7 Technology Environmental Health (EH&S) and Safety Risk Assessment
- Task 2. Community Benefits Plan (CBP)
- Task 3. Experimental Work/Validation
- Task 4. Process Design
- Task 5. Design of the DAC Contactor
- Task 6. Heat Integration and Thermal Management



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