Integrated Process for Direct Air Capture of CO$_2$ and Electrochemical Conversion to Ethanol

TCF-20-20118

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National Energy Technology Laboratory
Direct Air Capture Kickoff Meeting
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Program Overview

Funding: $1.5 mil/3 yrs (FE) + $1.5 mil in-kind match-up (ReactWell)

Overall Project Performance Dates: Jan 2021-Jan 2024

Project Participants: Radu Custelcean, Costas Tsouris, Kashif Nawaz (ORNL); Brandon Iglesias (ReactWell)

Overall Project Objectives: Develop an energy-efficient, cost-effective, net-zero emission technology that closes the carbon cycle by combining DAC with catalytic electrochemical conversion of CO$_2$ into ethanol

- DAC with aqueous amino acids and crystalline guanidine solids (ORNL)
- Electrochemical conversion of CO$_2$ into ethanol with Cu nanoparticles/carbon nanospike catalyst (ReactWell)
- Ethanol commercialization as hand sanitizer, spirits & fuel (ReactWell)
Technology Background

**Phase-change DAC process** – combines the benefits of aqueous solvents and solid sorbents

**DAC cycle**

- **Release**
  - $80 - 120 \, ^\circ C$
  - $\text{CO}_2$
  - $5 \, \text{H}_2\text{O}$

- **Absorption**
  - $\Delta H = 223 \, \text{kJ/mol}$
  - $\text{H}_2\text{O}: 148 \, \text{kJ/mol}$

- **Benchmark:**
  - $\text{CaCO}_3: 179 \, \text{kJ/mol, 900} \, ^\circ \text{C}$

**PyBIG-CO$_3$:** $K_{sp} = 1.0 \times 10^{-9}$

**CaCO$_3$:** $K_{sp} = 3.4 \times 10^{-9}$

**DAC bi-cycle with amino acid/PyBIG**

- $\text{CO}_2$
- $\text{H}_2\text{N}$
- $\text{PyBIGH}_2(\text{CO}_3)(\text{H}_2\text{O})_4(s)$
- $\Delta (80-120 \, ^\circ \text{C})$

**Angew. Chem. Int. Ed.** 2017, 56, 1042
- (highlighted in USA Today, Forbes)

**Nature Energy** 2018, 3, 553
- (top 5 story from Office of Science)

**Chem** 2019, 5, 719 (highlighted in Science)

**IUCRJ** 2019, 6, 56.

**Ind. Eng. Chem. Res.** 2019, 58, 23338

**ChemSusChem** 2020, 13, 6381

Technical Approach/Project Scope

Key milestones
1) DAC chemistry optimization
2) Contactor design, manufacturing, testing
3) Optimization of sorbent regeneration/CO₂ release
4) Process engineering & intensification
5) Atmospheric water capture
6) CO₂ conversion to ethanol
7) TEA and LCA
8) Technology scale-up and commercialization

Cu nanoparticle/carbon nanospike catalyst invented at ORNL, licensed to ReactWell 2019 R&D 100 Award
Team and Facilities

ORNL

Radu Custelcean
organic chemist

Costas Tsouris
chemical engineer

Kashif Nawaz
mechanical engineer

Diana Stamenova
organic chemist

Abishek Kasturi
grad student (Georgia Tech)

ReactWell

Brandon Iglesias
chemical engineer

Chem Chip catalyst

Carbonate analyzer
Progress and Current Status

DAC Chemistry: Identify the optimal amino acid/BIG combinations and reaction conditions leading to fastest rate of CO$_2$ absorption, highest cyclic capacity, and lowest regeneration energy.

Preliminary results (MGBIG/SAR): Catalytic amount of amino acid (10 mol%), no KOH, enhanced crystallization yield (from 28% to 84%), intensified 3-phase (gas+liquid+solid) process.
Opportunities for Collaboration

Internal collaborations
Synergy between BES (sorbent design & synthesis, structural analysis, thermodynamics) and FE (process optimization, scale up, commercialization)

External collaborations
Electrochemistry (solvent regeneration, CO\textsubscript{2} to EtOH conversion)
Membrane contactors (reactive membrane crystallization)
Industrial crystallization (controlling crystal form, nucleation & crystal growth, crystal morphology, particle size distribution)