

Integrated Process for Direct Air Capture of CO₂ and Electrochemical Conversion to Ethanol

TCF-20-20118

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Oak Ridge National Laboratory

ReactWell, LLC

U.S. Department of Energy

National Energy Technology Laboratory

Direct Air Capture Kickoff Meeting

February 24-25, 2021



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

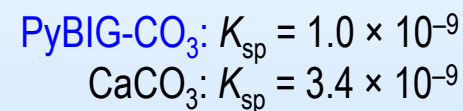
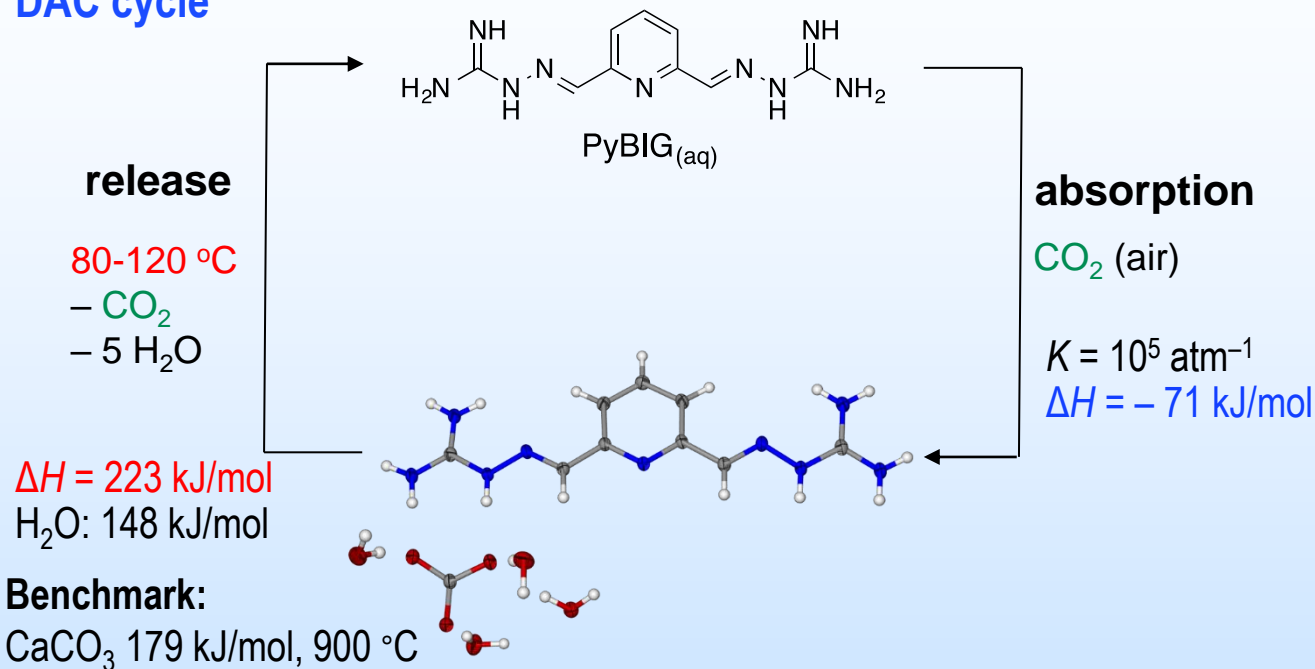
Project Participants: Radu Custelcean, Costas Tsouris, Kashif Nawaz (ORNL); Brandon Iglesias (ReactWell)

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 CO₂ into ethanol

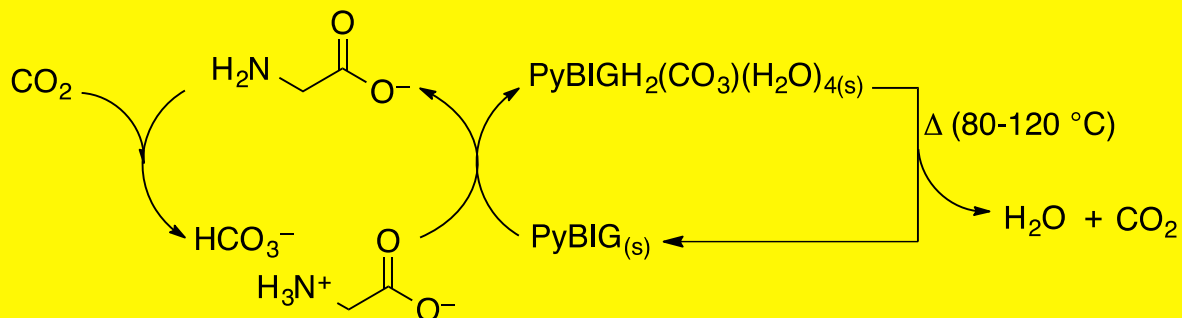
- DAC with aqueous amino acids and crystalline guanidine solids (ORNL)
- Electrochemical conversion of CO₂ into ethanol with Cu nanoparticles/carbon nanospike catalyst (ReactWell)
- Ethanol commercialization as hand sanitizer, spirits & fuel (ReactWell)

Technology Background

DAC cycle



DAC bi-cycle with amino acid/PyBIG

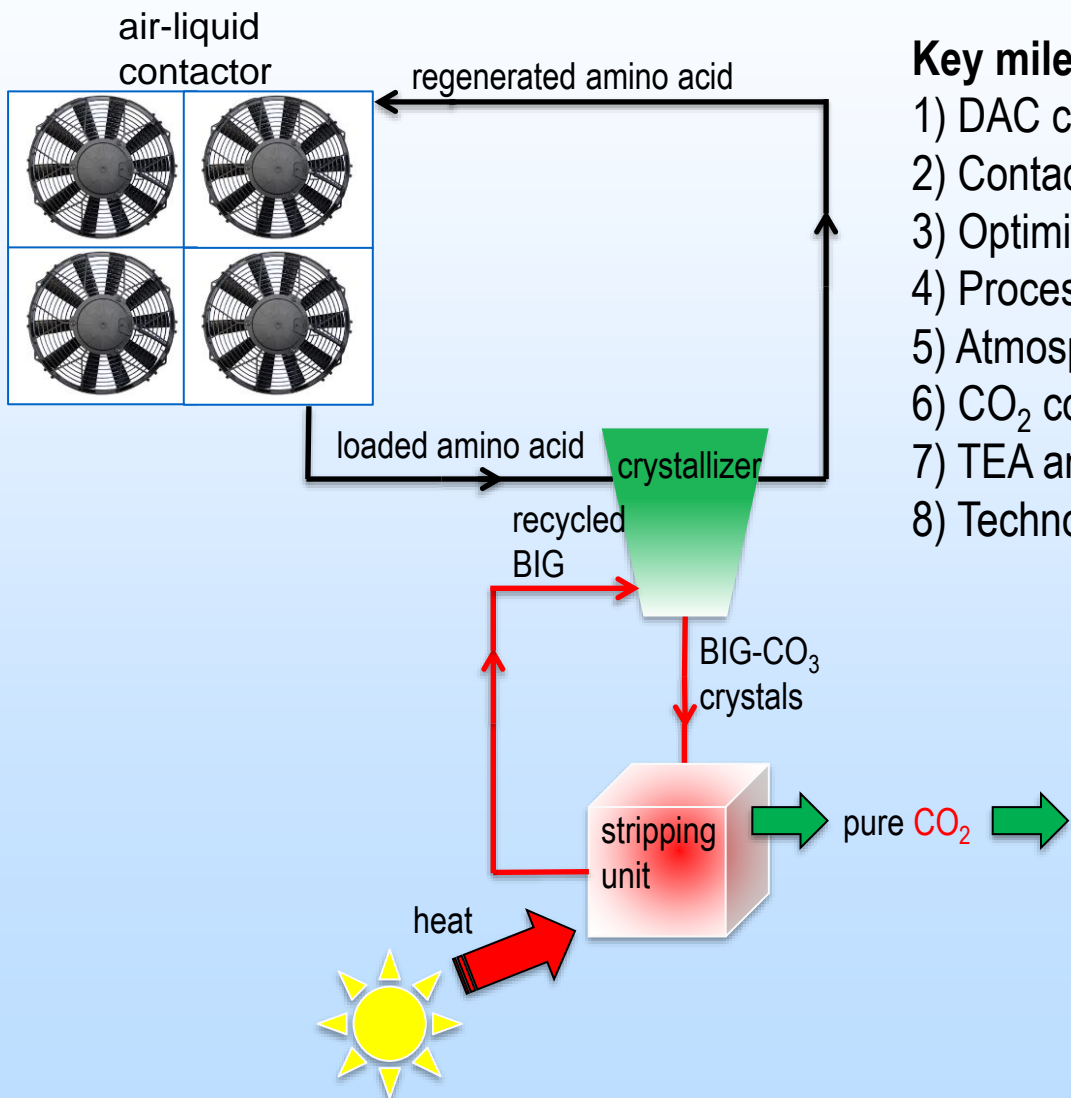


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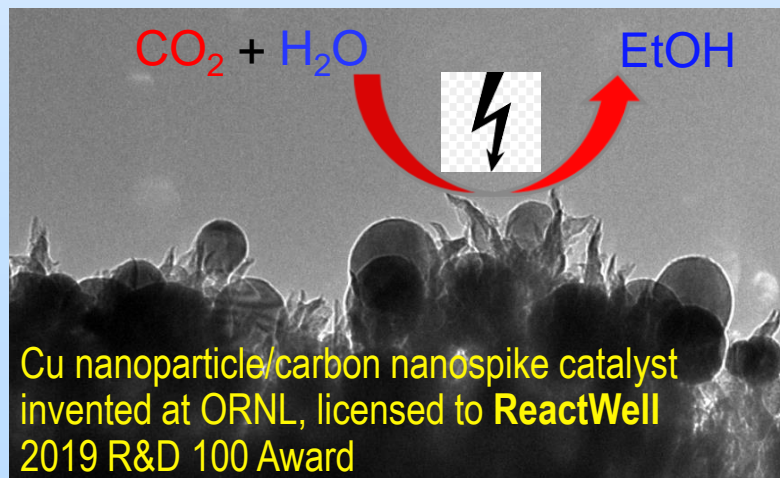
Phase-change DAC process – combines the benefits of aqueous solvents and solid sorbents

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



Team and Facilities

ORNL



Radu Custelcean
organic chemist



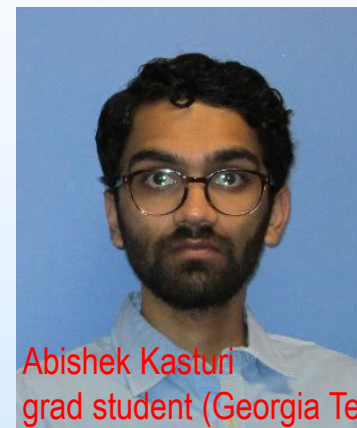
Costas Tsouris
chemical engineer



Kashif Nawaz
mechanical engineer



Diana Stamberga
organic chemist



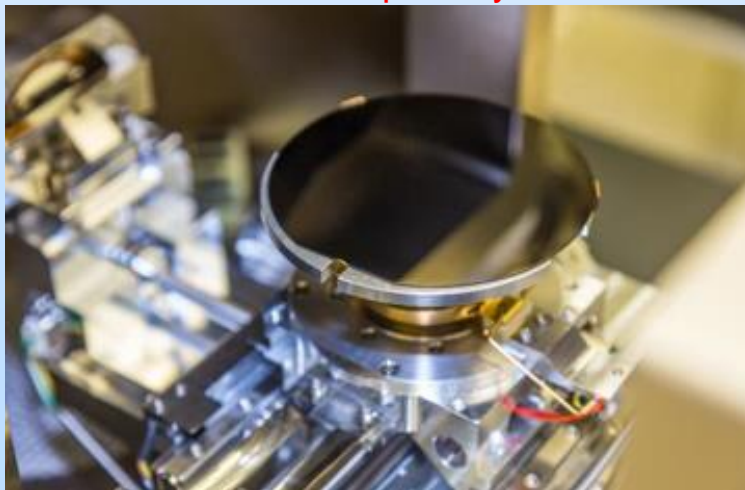
Abishek Kasturi
grad student (Georgia Tech)

ReactWell

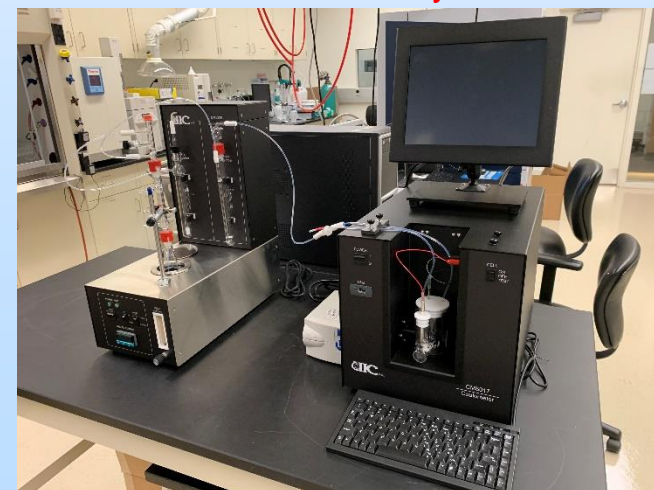


Brandon Iglesias
chemical engineer

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 CO₂ absorption, highest cyclic capacity, and lowest regeneration energy.

CO₂ absorption cycle:

$$\text{CO}_2 + \text{BIG-K} \rightleftharpoons \text{BIGH}_2\text{-CO}_3 \xrightarrow{\text{heat}} \text{H}_2\text{O} + \text{CO}_2 + \text{BIG}$$

PyBIG

Nc1cc(NC(=O)N)nc(NC(=O)N)c1

m-BBIG

Nc1ccc(NC(=O)N)cc(NC(=O)N)c1

MGBIG (0.5 M)

Nc1nc(NC(=O)N)nc(NC(=O)N)c1

SAR (0–0.5 M)

NCC(=O)O

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, CO₂ to EtOH conversion)

Membrane contactors (reactive membrane crystallization)

Industrial crystallization (controlling crystal form, nucleation & crystal growth, crystal morphology, particle size distribution)