Award Number: DE-SC0023939
Business contact: mitch.odinak@moleculeworks.com

MoleculeWorks
Efficiency for a Sustainable World

Direct air capture of carbon dioxide and production of oxygenated hydrocarbons in one unit operation system

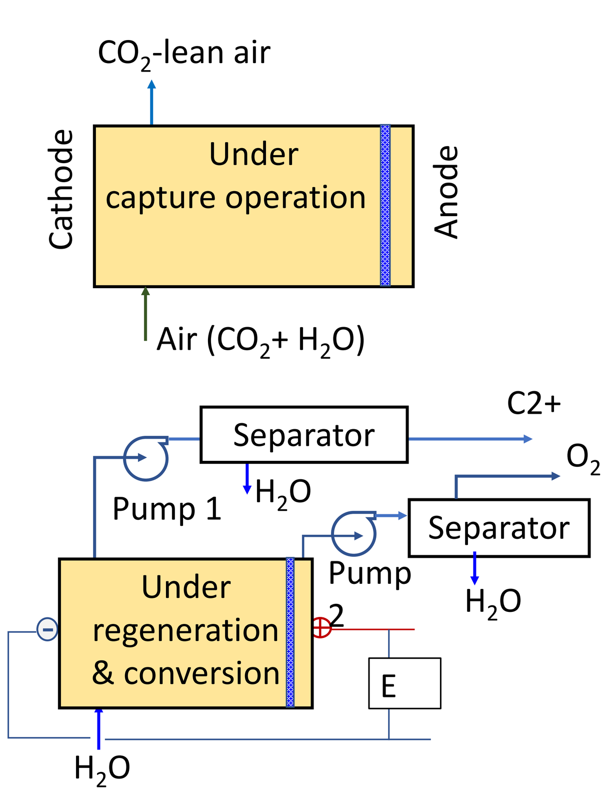
PI: Wei Liu/wei.liu@moleculeworks.com

I. The project goal

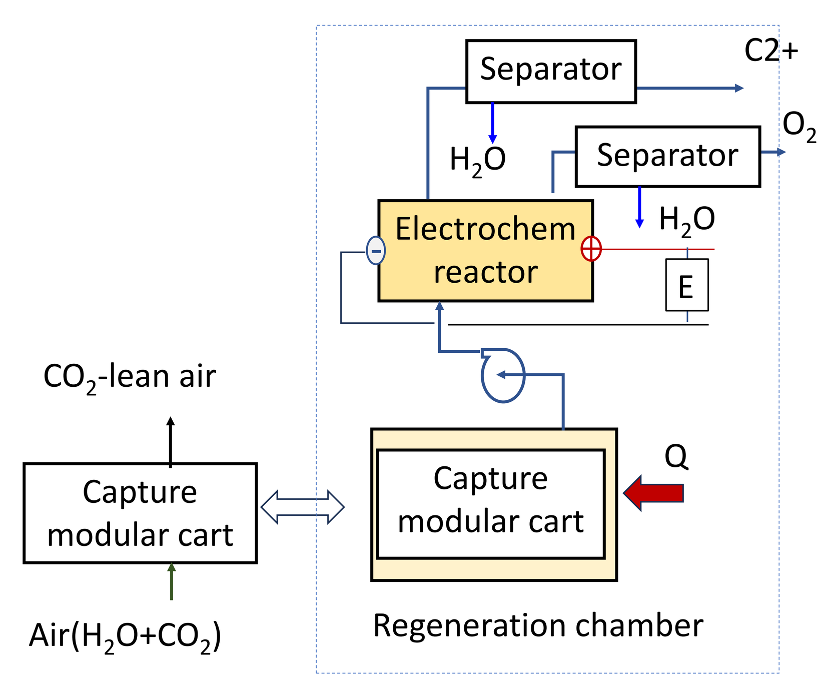
- Integrate direct air capture of carbon dioxide by solid adsorption with conversion to C2+ oxygenate hydrocarbons as one unit operation system, using renewable electricity.
  - The C2+ oxygenates, including ethanol, acetate, propanol, and acetone, can be used as oxygenated fuels, upgraded to jet fuels, or separated into individual chemical products.
- Make the unit to be deployable anywhere cheap electricity is available to convert CO_2 and H_2O from air into liquid products without any additional feedstock.

II. Process integration approach and technology innovations

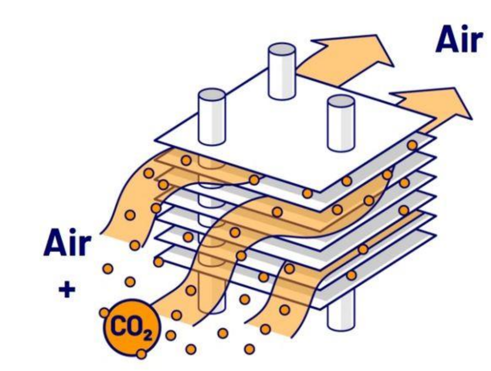
I. Integrating capture, regeneration, electrochemical conversion into one unit cell



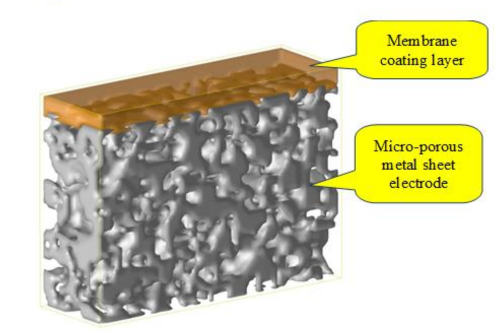
II. Integrating regeneration and electrochemical conversion into one unit operation



1. Molecule Works' adsorption/heat exchange (AHX) reactor designs for direct air capture with low cost and low energy consumption
   https://cleancapturetech.com/

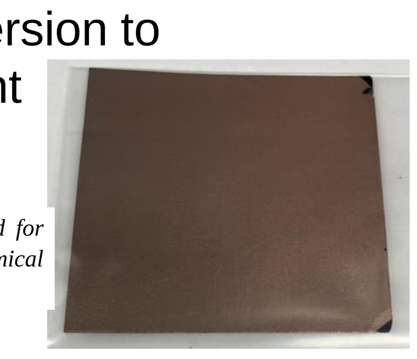


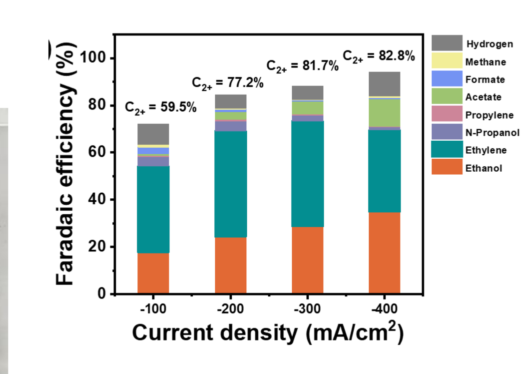
2. Molecule Works' porous zirconia/Nickel alloy sheet as anodic membrane electrode assembly (MEA) with thermal and chemical durability



3. ANL's (Dr. DJ Liu's team) cathodic catalysts for CO_2 +H_2O conversion to C2+ oxygenates with excellent productivity and selectivity

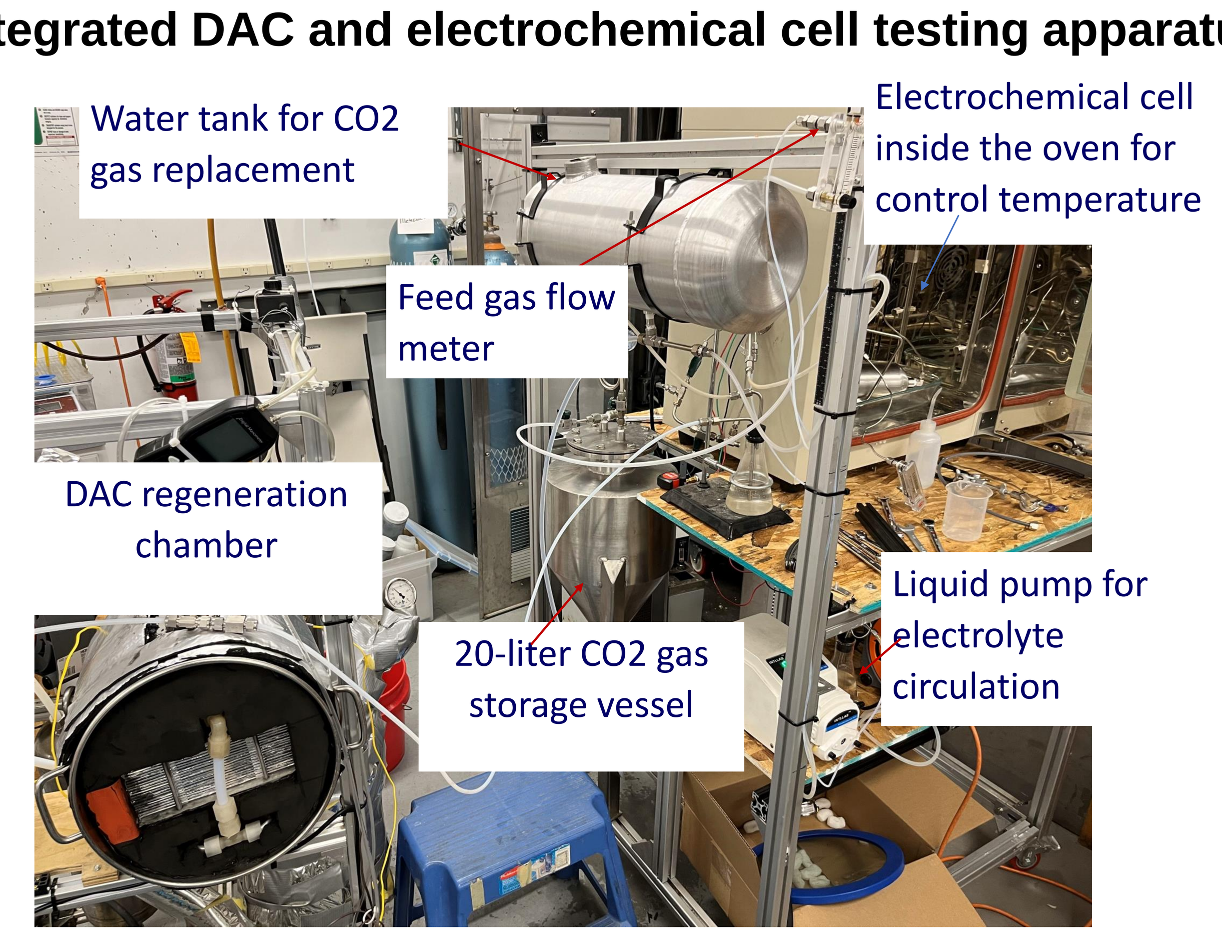
DJ. Liu, T. Xu, H. Xu and D. Rebollar, "Versatile Method for Preparing Highly Effective Electrocatalyst for CO2 to Chemical Conversion" ***R&D 100 Award, 2020.***



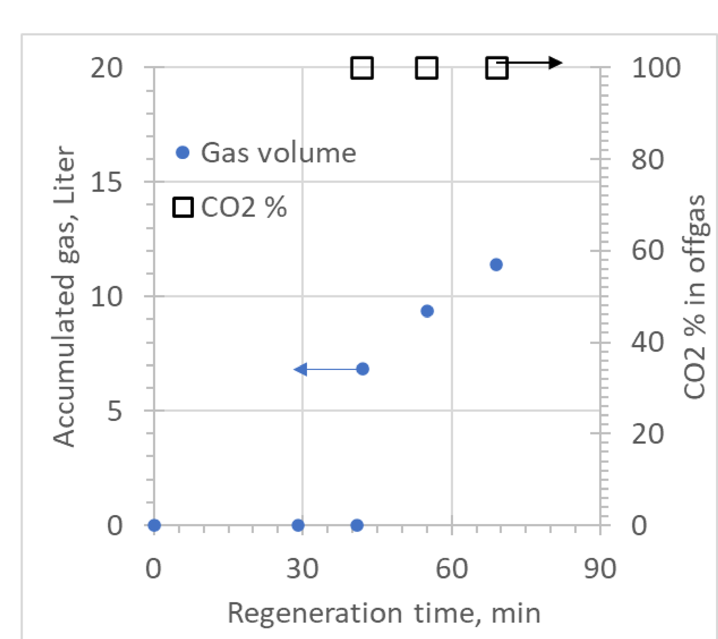


III. Phase I experimental results

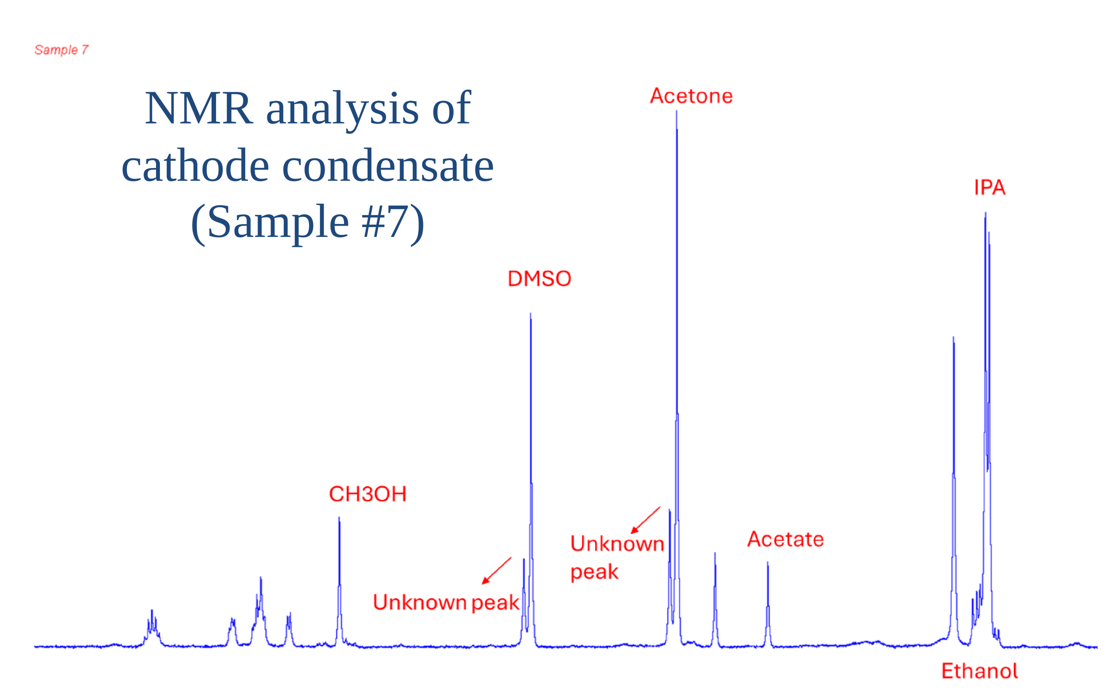
Integrated DAC and electrochemical cell testing apparatus



>95% CO_2 can be produced by regenerating the adsorbent with hot water heating and rough vacuum pulling

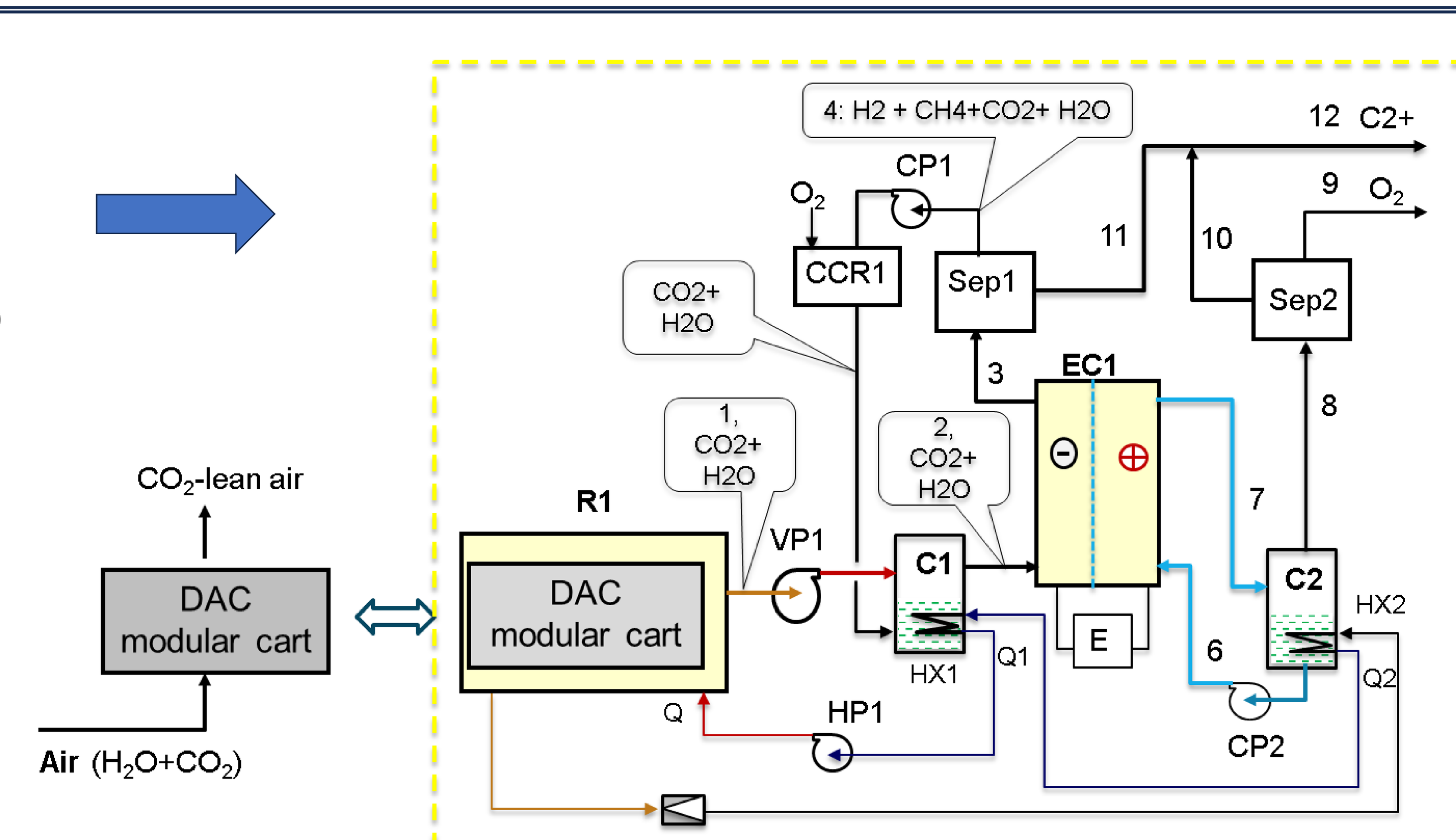


Significant amounts of C2 and C3 oxygenates are produced with the DAC CO_2 at voltage of 2.0 – 2.5V and temperatures of 50 to 80ºC under atmospheric pressure



IV. Success

- Feasibility of integrating DAC with conversion of CO_2 into C2+ oxygenates as *one unit operation system* is demonstrated.
- CO_2 produced by adsorption-based DAC process can be used directly as a feed to the electrochemical cell with performances same or comparable to the CO_2 from beverage grade cylinder.
- The electrochemical cell (EC) can be conducted at temperatures close to regeneration offgas temperature, beyond room temperature.
- EC cell assembled from ANL's cathode catalyst (Cu/carbon) and Molecule Works ceramic/nickel sheet showed stable performance with current density above 100 mA/cm^2 at 2.5V in 3-day testing.



V. Challenges

- The EC cell must be assembled with durable materials that are resistant to organic solvent, temperature, and electrical heating
- The product is a mixture, and large product samples need to be produced for C balances.
- Electrical efficiency is a major cost factor, and efficiency to C2+ portion of the products need to be optimized

Acknowledgement

- Dr. DJ Liu at ANL for making and characterizing the cathode catalyst as well as product analysis by NMR technique
- DOE SBIR office and program manager (Dr. Richard Bergen)