# Bench-Scale Testing of Monolithic Poly(Propyleneimine) Structured Contactors for Direct Air Capture of Carbon Dioxide

### primary project goal

CORMETECH Inc., in partnership with Global Thermostat LLC and Georgia Institute of Technology, is developing and testing a novel sorbent-air contactor composition with low pressure drop optimized for carbon dioxide (CO<sub>2</sub>) removal from ambient air. The project is focused on optimizing a monolith contactor to support a next-generation sorbent composition, linear poly(propyleneimine) (I-PPI), which offers advantages over benchmark poly(ethyleneimine) (PEI)-based sorbents for direct air capture (DAC). The novel approach will maximize the volumetric productivity of the DAC process while reducing the auxiliary power required to capture  $CO_2$  from air.

#### technical goals

- Perform experimental and simulation studies of the novel CO<sub>2</sub> sorbent/gas contactor system based on I-PPI sorbents at DAC-relevant conditions.
- Measure isotherm, kinetic, and transport behaviors of the powder and slab materials.
- Develop a single channel monolith model to optimize the geometry and the meso/macro-porosity of monoliths specifically tuned for I-PPI.
- Develop a transport model based on I-PPI supported on monolith slabs.
- Build and evaluate a single brick sorption tester (SBST) for the bench-scale evaluation of extruded monoliths loaded with I-PPI, enabling the CO<sub>2</sub> sorption performance to be optimized.
- Measure the resistance of the sorbent/contactor composition to oxidation under relevant dry and humid conditions.
- Perform a techno-economic analysis (TEA) utilizing the process model incorporating the novel sorbent/contactor combination.

#### technical content

Global Thermostat's baseline DAC process employs monolithic, low pressure drop contactors loaded with organic amine molecules or macromolecules to allow for high throughput gas/solid contacting with high volumetric  $CO_2$  sorption productivity. The Global Thermostat DAC process employs relatively shallow honeycomb monolith contactors (~15 cm deep) that permit low pressure drops (hundreds of Pa) at gas approach velocities of 3–5 m s<sup>-1</sup> while still maintaining a high geometric surface area per unit volume (Figure 1).

## program area:

Carbon Dioxide Removal

ending scale: Bench Scale

application: Direct Air Capture

key technology: Sorbents

#### project focus:

Monolith Contactor Impregnated with Novel Sorbent for DAC

participant: CORMETECH Inc.

project number: FE0032094

predecessor projects: N/A

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#### partners:

Georgia Institute of Technology; Global Thermostat LLC

start date: 09.15.2021

percent complete: 15%



Figure 1: Monolith system used in Global Thermostat process.

After CO<sub>2</sub> adsorption, CO<sub>2</sub> is desorbed and collected by combined temperature-vacuum swing desorption employing steam-stripping, producing a concentrated CO<sub>2</sub> product (Figure 2). Early generations of Global Thermostat's technology used commercially available components that were initially designed and optimized for other applications (e.g., [i] nonporous monolithic contactors with porous oxide washcoats designed for high-temperature catalytic applications and [ii] known commercially available amine compositions). Whereas commercially available materials were leveraged in early development, this project is focused on design and optimization of a gas/solid contactor specifically formulated for DAC.



Figure 2: CO<sub>2</sub> desorption using steam regeneration.

Recently, Global Thermostat has developed several generations of amine sorbents with improved properties for DAC in collaboration with Georgia Tech, relative to a baseline commercial amine composition, PEI. Global Thermostat also has collaborated closely with CORMETECH to design and formulate new porous monolith contactors specifically engineered to support PEI amine compositions for DAC. The purpose of this current project is to advance the design of a new

monolithic air/solid contactor by developing designs optimized specifically for DAC by tailoring the properties of the monolith contactor to fit synergistically with the next-generation amine composition, I-PPI. The benchmark amine polymer, PEI, is deployed as a branched oligomer. In contrast, the selected next-generation polymer is linear in structure (I-PPI). Given the different structure of the macromolecule (PEI: branched with ethyl linkers, versus I-PPI: linear with propyl linkers), the new polymer can be expected to interface with the porous monolith support differently from the baseline PEI case. In powder tests (data are shown in Figure 3), I-PPI has similar CO<sub>2</sub> sorption properties as PEI, yet superior oxidative stability and water sorption properties (more hydrophobic), making it a promising next-generation amine polymer for DAC. Furthermore, I-PPI has recently been scaled up to the 100-gram quantity levels by project partner Celares GmbH, who is providing sufficient quantities of the polymer needed for monolith-scale testing. Given the promise of I-PPI as a sorbent composition, the focus of this project is to customize a monolith formulation for this next generation sorbent. The project is directed at conducting experimental measurements and formulating a sorption/diffusion/transport model of the adsorption process, which can be used to advance process models and inform process TEAs.



Figure 3. Left: Isotherms at varied temperatures for PPI/SBA-15 sorbents. Right: Amine efficiency versus amine loading for I-PPI versus PEI (closed shapes), 400 ppm CO<sub>2</sub> at 35°C, showing loss after treatment in oxidative environment (open shapes), 21%O<sub>2</sub>/N<sub>2</sub>, 110° C for 24 hours.

#### technology advantages

- Monolithic contactor achieves low pressure drop CO<sub>2</sub> capture capability.
- New sorbent with enhanced oxidative stability will improve the on-steam sorbent lifetime in the base Global Thermostat DAC process.
- Utilizes cost-effective fabrication technique from CORMETECH for CO<sub>2</sub> contactor development using porous monolith substrate that can be impregnated with the amine.

#### **R&D** challenges

- Synthesis of I-PPI sorbent at kg-scale for full-size optimized monolith brick impregnation and SBST validation testing.
- Development of single-channel monolith with combined momentum, mass, and heat transfer, incorporating porous wall flow and the multi-phase regimes that arise from the use of steam as a desorbing medium, to optimize the monolithic substrate's textural properties for I-PPI and maximize DAC performance.
- Measurement of fundamental transport properties of CO<sub>2</sub> through amine-loaded porous materials and adsorption/desorption equilibria, for model development and incorporation into the single channel monolith model.
- Confirmation of the enhanced oxidative stability of the scaled-up I-PPI sorbent.

#### status

The project team is currently designing, building, and commissioning the bench-scale SBST unit, along with manufacturing, validation, and bench-scale testing of I-PPI (at kg-scale) using a standard monolithic substrate and the SBST. Development of a single channel model to optimize the geometry and the meso/macro-porosity of monoliths specifically tuned for I-PPI is being conducted. Ongoing efforts include measurement of the adsorption isotherms, kinetic, and transport behaviors of I-PPI, supported on powder and on slab materials to develop an adsorption model and a transport model for inclusion in the single channel monolith model. The process model is also being updated to incorporate the novel sorbent/contactor combination to support the TEA for larger-scale applications.

#### available reports/technical papers/presentations

Christopher Bertole, "Bench-Scale Testing of Monolithic Poly Propyleneimine Structured Contactors for Direct Air Capture of Carbon Dioxide," Project kickoff meeting presentation, Pittsburgh, PA, October 2021. http://www.netl.doe.gov/projects/plp-download.aspx?id=12444&filename=Bench-Scale+Testing+of+Monolithic+Poly+Propyleneimine+Structured+Contactors+for+Direct+Air+Capture+of+Carbon+Dioxi de.pdf.