



the **ENERGY** lab

## R&D FACTS

### Carbon Capture

## Carbon Capture Research and Development

Carbon capture and storage from fossil-based power generation is a critical component of realistic strategies for arresting the rise in atmospheric CO<sub>2</sub> concentrations, but capturing substantial amounts of CO<sub>2</sub> using current technology would result in a prohibitive rise in the cost of producing energy. The National Energy Technology Laboratory-Office of Research and Development (NETL-ORD) is pursuing a multifaceted approach, which leverages cutting-edge research facilities, world-class scientists and engineers, and strategic collaborations to foster the discovery, development, and demonstration of efficient and economical approaches to carbon capture.



*Integrated technology development takes materials from molecular design through fabrication to commercialization.*

### Project Overview

The NETL-ORD capture program seeks to create technological solutions for carbon capture from pulverized coal power plants and integrated gasification combined cycle (IGCC) plants. Capture conditions are vastly different in each of these power cycles, so separate materials development programs have been undertaken for each. Additionally, both the IGCC and oxy-fuel cycles require large amounts of oxygen, which is expensive to produce and adds considerable cost to the processes.

Three approaches have generally been considered for the separation of CO<sub>2</sub> in power generation applications. Sorbents are solid materials which selectively sorb CO<sub>2</sub> from gas mixtures and release it after a change in either temperature or pressure, producing a pure stream of CO<sub>2</sub>. Solvents are liquid materials which function in a similar fashion. Membranes are devices which allow CO<sub>2</sub> to pass through and retain all the other components of gas mixtures. Each technology has its own advantages and disadvantages.

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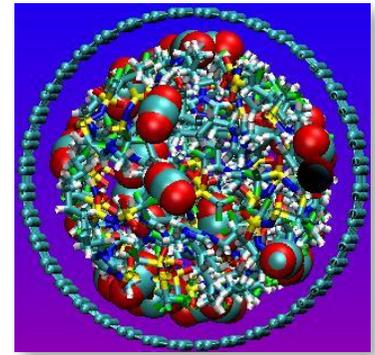
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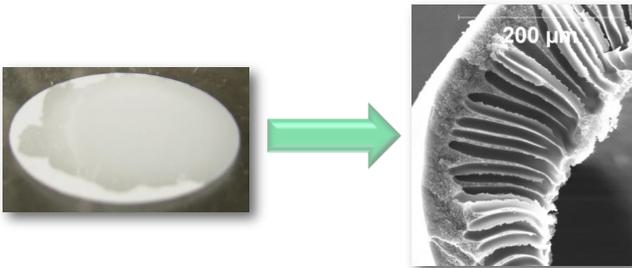
Generally, solvents are the best understood technologies, and the existing commercial products for CO<sub>2</sub> capture are all solvent-based (Selexol, Rectisol, MEA). Sorbents and, particularly, membranes are less developed as CO<sub>2</sub> capture technologies but have the potential for much greater improvements in performance compared to existing technologies. NETL-ORD is examining all three classes of technologies to better address both near and longer term capture goals.

To accelerate development of solvents, sorbents, and membranes, NETL-ORD is pursuing the complimentary utilization of computational and experimental approaches. For example, atomistic modeling approaches are coupled with surface science experiments to understand and optimize the structure and energetics of materials for the specific application. The resulting molecular-level information can be used as a basis to predict the bulk thermodynamic and kinetic material properties by force-field modeling, Monte Carlo simulation, and molecular dynamics. Validated models are used to predict the performance of materials in the application of interest, thus allowing experimental resources to focus on only the most promising materials. Substances designed using fundamental approaches are synthesized and characterized in NETL-ORD's fully equipped synthetic facilities, and the materials are fabricated into configurations, including thin-film membranes and sorbent particles, to assess their performance at conditions consistent with those encountered in carbon dioxide capture applications.



*Computational models examine the molecular level interactions of materials and aid in optimization.*

Researchers work closely with process analysts to provide high quality information required for techno-economic assessments to minimize the erroneous assumptions that are often required when extrapolating laboratory results to plant-scale models. Laboratory results are scaled to the device level, such as a membrane module or sorbent bed, using a combined experimental and computational approach. In this approach, computational fluid dynamics and small-scale device fabrication and testing work hand-in-hand to provide insights into the functional performance that can be expected at the plant scale, including performance degradation and heat- and mass-transfer limitations. The integrated approach, which can be envisioned as a cyclic process ranging from fundamental science through process evaluation, results in an accurate assessment of emerging technologies being developed. Furthermore, this process provides researchers insight into the properties that must be improved in future generations of materials and the scientific limitations bounding technologies. The close relationship of the scientists, engineers, and systems analysts allows each step in the technology development approach to continuously inform the others and produce greater efficiency. This approach continues to provide rapid advancement in the development of several materials including amine-enriched sorbents, ionic liquids, and metal-organic frameworks.



*Advanced fabrication and synthetic techniques move conceptual materials toward practical application.*

## Expected Outcomes

The most promising materials, those which appear likely to achieve substantial reductions in the cost of carbon capture, will be further tested at the National Carbon Capture Center or other power generation facilities using actual flue or fuel gas. Technologies, which test favorably under these conditions, will be transferred to industry through joint development and patent licensing. The research described will result in the creation of new materials, characterization of the performance of the materials under realistic conditions, and accelerated commercialization of technologies based on the materials.

## Benefits

The research will accelerate the development (ranging from the discovery of innovative materials through evaluation in real systems) of efficient, cost-effective fossil fuel conversion systems that meet the programmatic goals for CO<sub>2</sub> capture. Materials and separation technologies developed in this research may also have impacts in other areas such as natural gas purification.