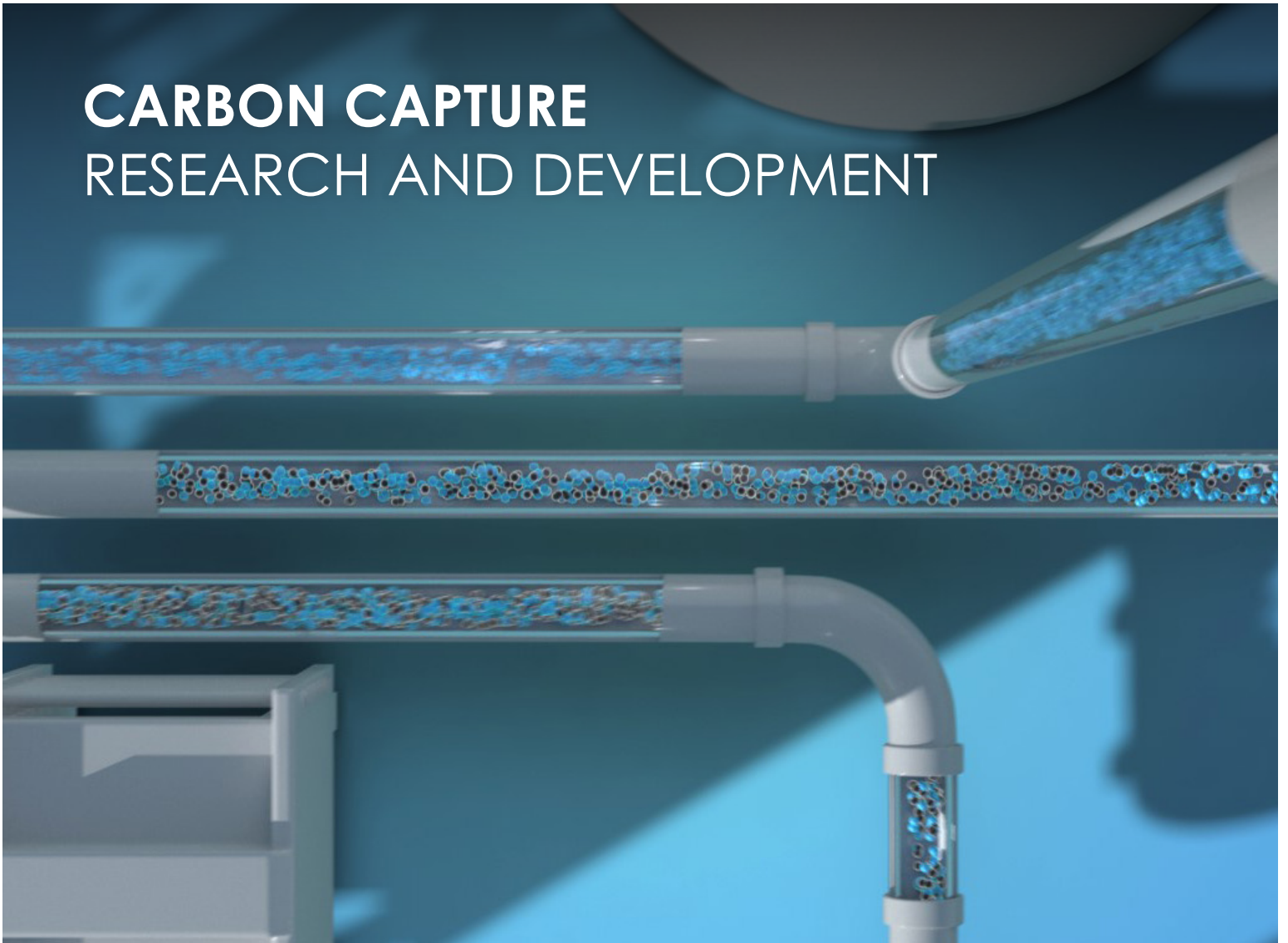


# CARBON CAPTURE RESEARCH AND DEVELOPMENT



# NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

## PROJECT OVERVIEW

The NETL Carbon Capture Program is creating technological solutions for carbon capture from natural gas or pulverized coal (PC) power plants, as well as emerging applications such as: hydrogen production from steam methane reforming; industrial point sources such as cement and steel production; and direct air capture. The capture conditions are vastly different in each of these applications. Therefore, separate materials development programs have been undertaken for each.

Three approaches have traditionally been considered for the separation of CO<sub>2</sub> in power generation applications. Sorbents are solid materials that 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 that function in a similar fashion. Membranes are devices that selectively split process streams into CO<sub>2</sub>-rich and CO<sub>2</sub>-depleted streams. Each technology has advantages and disadvantages, and each emerging application may utilize one or more technologies to achieve economical separations.

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

NETL researchers tackle the most challenging carbon capture problems using a holistic approach. Researchers begin with computer modeling, move on to material fabrication, then to device fabrication. They complete the cycle with process analysis and to field testing. Computational approaches are utilized to identify new materials and combinations of materials that offer distinct performance advantage over existing materials. This is accomplished through: atomistic modeling; molecular dynamics simulations; Grand Canonical Monte Carlo simulations; and applying machine learning algorithms on a material performance database. One such approach for computational screening of solvents has led to the identification of a new, previously overlooked solvent for carbon capture with its performance validated through field testing with our partner organizations. Currently, new computational methods are being developed to improve the prediction of the properties of metal organic frameworks (MOFs) and polymers for gas separations.

NETL researchers also utilize the Functional Materials Synthesis Laboratory to fabricate new materials and to perform standard laboratory tests to validate their performance, both under idealized conditions and under process conditions. Some of our recent experimental research materials include: amine sorbents embedded into polymer films, MOF sorbents, porous polymer sorbents and membranes, ion gel membranes, and amine-functionalized facilitated transport membranes. While many research groups have looked at these materials from a fundamental perspective, NETL researchers are taking a step further to help enable commercial adoption of these technologies through device fabrication and access to field testing resources through our partner institutions. For instance, we pursue the pelletization of sorbents, and the fabrication of ultra-high permeance membranes through porous support development and refinements in thin film coating techniques. Through our partnership with the National Carbon Capture Center, we are operating and expanding test equipment that enables material and device testing using real flue gas from a coal-fired boiler, as well as a natural gas boiler.

Researchers work closely with process analysts to provide high-quality information required for techno-economic

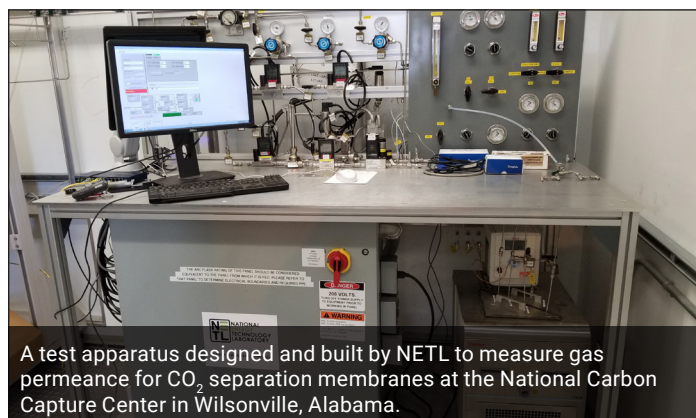
assessments of plant-scale models. Laboratory results are scaled to the device level, such as a membrane module or sorbent bed, using a combined experimental and computational approach. Computational fluid dynamics and small-scale device fabrication work hand-in-hand to provide insights into the functional performance that can be expected at the plant scale, including performance degradation and heat- and mass-transfer limitations. Systems analysts at NETL work to integrate innovative materials and devices into optimized carbon capture systems, and to predict the cost of capture for the complete process. Feedback shared between scientists, engineers, and systems analysts allows each step in the technology development approach to continuously inform all stakeholders, resulting in greater efficiency.

## EXPECTED OUTCOMES

The most promising materials, those that appear likely to achieve substantial reductions in the cost of carbon capture, will be further tested at the National Carbon Capture Center or at other partner facilities using actual process streams. Technologies that 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 carbon capture 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 hydrogen production and natural gas purification.



A test apparatus designed and built by NETL to measure gas permeance for CO<sub>2</sub> separation membranes at the National Carbon Capture Center in Wilsonville, Alabama.

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### Research Partners

National Carbon Capture Center  
Leidos Research Support Team (LRST)