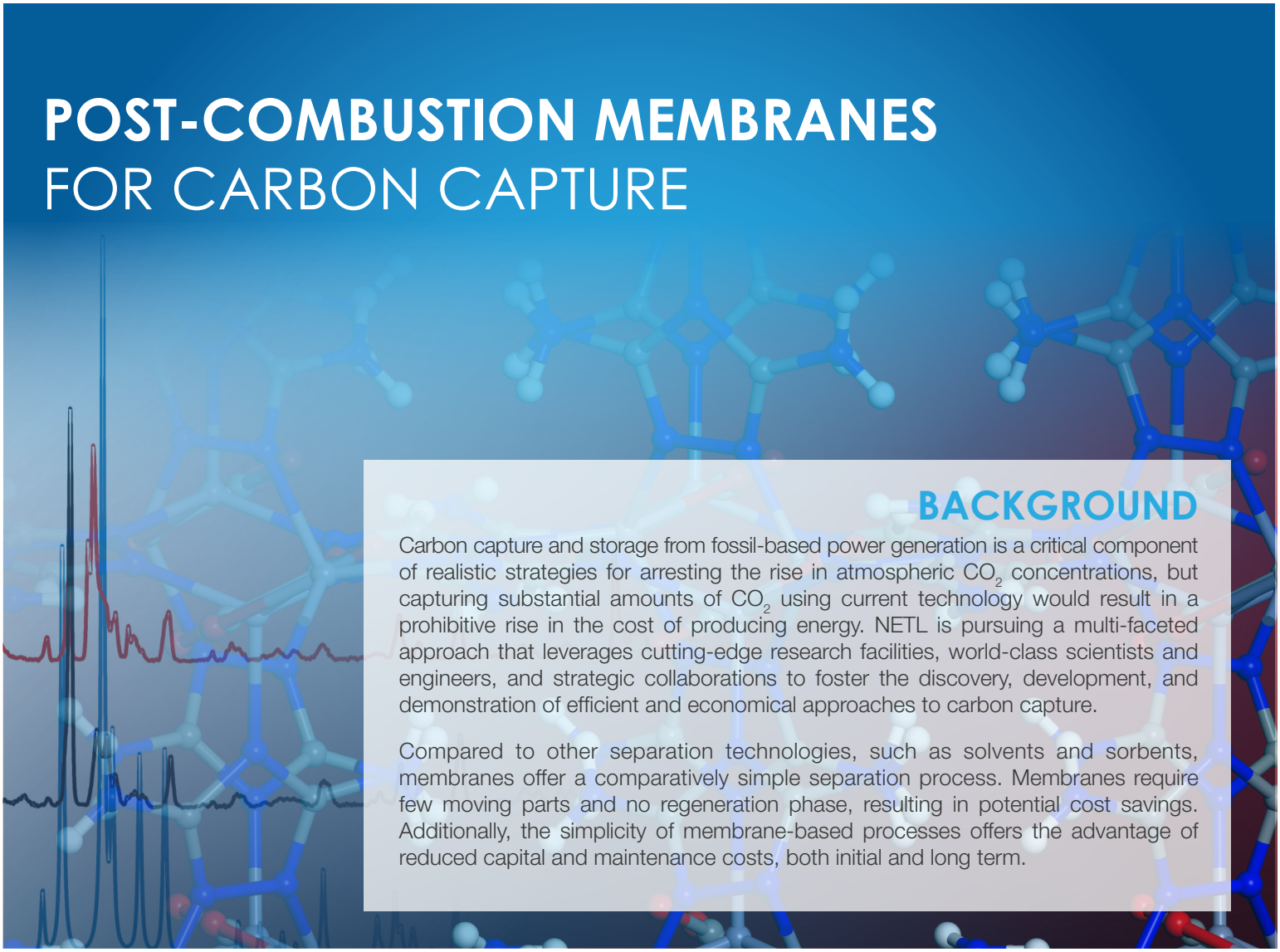
POST-COMBUSTION MEMBRANES FOR CARBON CAPTURE



BACKGROUND

Carbon capture and storage from fossil-based power generation is a critical component of realistic strategies for arresting the rise in atmospheric CO_2 concentrations, but capturing substantial amounts of CO_2 using current technology would result in a prohibitive rise in the cost of producing energy. NETL is pursuing a multi-faceted approach that 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.

Compared to other separation technologies, such as solvents and sorbents, membranes offer a comparatively simple separation process. Membranes require few moving parts and no regeneration phase, resulting in potential cost savings. Additionally, the simplicity of membrane-based processes offers the advantage of reduced capital and maintenance costs, both initial and long term.

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APPROACH

A typical flue gas stream contains less than 15 percent CO_2 and is only slightly above ambient pressure. This results in a very low driving force for membrane separation. Overcoming this lack of driving force requires highly permeable and highly selective membranes. Polymeric membranes are cheap and easy to process, but they are limited by an inherent tradeoff between permeability and selectivity. Polymeric membranes can have high permeability or high selectivity, but it is very difficult to achieve both. Conversely, metal organic frameworks (MOFs) are inorganic crystallite materials that show excellent potential for CO_2 capture. However, fabricating defect-free membranes solely from MOFs is very difficult and is hundreds of times more expensive than fabricating polymer membranes. Membrane material development by NETL focuses on mixed matrix membranes (MMMs), which are a class of materials consisting of inorganic crystalline particles (MOFs in this case) dispersed in a polymer matrix.

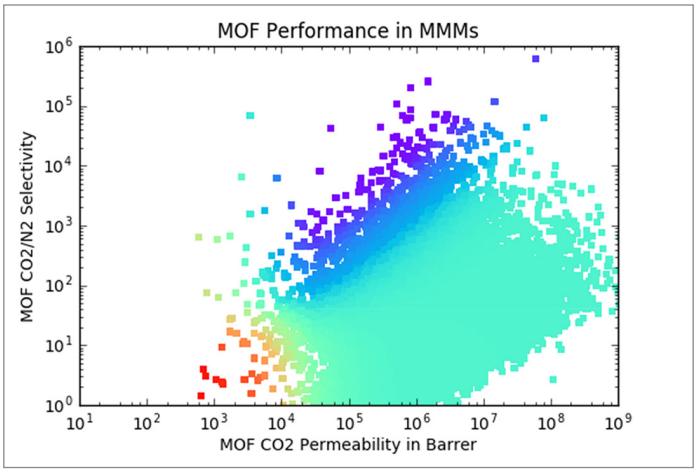
Properly-made MMMs combine the excellent process ability of polymers with the superior separation capability of the inorganic filler particles, making them a particularly attractive option for post-combustion carbon capture. Integrating filler particles into a polymer membrane can increase the membrane's selectivity and permeance while providing the fillers an efficient mechanism for contacting the feed-gas stream. In contrast to conventional polymer membranes, the MMM's increased selectivity and permeance allows the system to efficiently handle a low partial-pressure driving force. However, not all MOF particles are guaranteed to improve a polymer; to get the very best MMM from a given polymer, an appropriate MOF must be selected from thousands of possible MOFs. Overcoming this problem is key to developing MMMs that are defect-free and possess the separation characteristics necessary to meet DOE goals.

While the incorporation of filler particles into polymer membranes has the potential to lead to better membranes, an almost infinite variety of MOF filler particles exist, and it is important to choose MOF particles with properties that properly match the polymer. Low cost computational methods are preferred for screening MOF materials due to the availability of large databases of real and hypothetical MOF structures and the speed of high-throughput computational methods. In addition, the process design and process variables that are adopted together with the material will affect the cost of carbon capture (CCC) that results from using a given material. It is possible, given a suitable process design, to optimize the process conditions for several combinations of material characteristics to create an interpolated map that connects MMM structure to an estimated CCC.

ACCOMPLISHMENTS

NETL researchers are engaged in a large computational screening study of MMMs in which high-throughput simulations are used to generate selectivity and permeability data for many MOF particles. The study includes MOF structures that have already been synthesized, as well as hypothetical MOFs. This data can be combined with experimental data for polymer membranes to predict properties of a large number of novel MMMs. NETL conducted computational process optimization for a three-stage membrane CO_2 removal process at selected process variable values and interpolated the results to give an approximate cost of carbon capture (CCC) for each polymer-MOF combination in our database. In this way, a connection was made from atomistic simulations of MOF materials to process optimization and, ultimately, to the CCC for each polymer-MOF combination.

In the figure below, data are plotted for approximately 125,000 MOF materials. For each MOF, a dot appears at the CO_2/N_2 selectivity and CO_2 permeability that corresponds to that MOF. Each dot is assigned a color that corresponds to the CCC that our method predicts. (Red indicates high cost, green is middle cost, and purple is the lowest cost.) This data offers researchers the potential to create MMMs based on the most advantageous pairing of polymer and MOF properties.



Calculated selectivity versus CO_2 permeability for a large database of MOF materials. Each point is colored based on the relative cost of carbon capture predicted for a hypothetical mixed matrix membrane made using that MOF. Cost is highest for red, moderately high for green, moderately low for blue and low for purple.

EXPECTED OUTCOMES

Researchers will use the relationship between MOF structure, polymer property and projected CCC to select candidate MOFs to synthesize and incorporate into polymer membranes. This data will also allow researchers to understand more clearly the characteristics of MOFs that contribute the most dramatic improvement to polymer materials.

Membrane technologies will be developed and evaluated under realistic testing conditions at successively larger scales, with eventual bench-scale testing in the presence of real fuel gas at the National Carbon Capture Center, sponsored by the U.S. Department of Energy.

BENEFITS

This research will accelerate the development of efficient, cost-effective fossil fuel conversion systems that meet the goal of capturing 90 percent of the CO_2 produced by a pulverized coal power plant at a cost of less than $40/tonne CO_2. This effort will range from the discovery of innovative materials through evaluation in real systems.

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