

## Introduction to CO<sub>2</sub> Capture

The generation of carbon dioxide is a direct consequence of extracting the maximum energy possible from fossil fuels. However, emissions of CO<sub>2</sub> to the atmosphere can be avoided by returning the carbon to the lithosphere. At sufficient purity, CO<sub>2</sub> can be injected into the subsurface for permanent storage (see section 2.5 of this report). However, because fuel conversion requires oxygen from the environment, at least one chemical separation must be performed to achieve the CO<sub>2</sub> purity required.

Carbon dioxide capture and separation is a costly and inefficient process using present day technology. At thermodynamic efficiencies of 15% - 25%, these unit operations can consume 10% - 20% of a power plant's output, and their use is predicted to raise electricity generation costs by 50 to 100%. There is significant opportunity to exploit fundamental advances in chemistry and engineering to drive down the operational penalties that CO<sub>2</sub> capture imposes on power production.

As a result of a targeted solicitation in 2012, GCEP has five projects in the area of carbon capture and separation. Three of the projects are developing materials for pre-combustion or post-combustion carbon capture and separation. The other two projects are systems analysis efforts to define optimum design and performance parameters for various capture technologies, including those funded. Research at some of the external institutions did not begin until 2013.

A multi-disciplinary team led by Jennifer Wilcox at Stanford is involved in the “Surface Functionalization of Mesoporous Silica-Based Sorbents for Capture”. The researchers are developing high surface area carbon-based materials that have been functionalized with model complexes of carbonic anhydrases. To date, they have developed and evaluated two types of dendritic amines and will continue this work as well as expanding towards Zn-functionalized groups. The amine functional groups have been loaded onto silica-based sorbents, with the ultimate goal of using mesoporous carbon frameworks. The group has synthesized a series of new mesoporous carbon materials and is studying the surface properties of those materials.

A team of researchers led by Randall Snurr at Northwestern University is examining metal organic frameworks (MOFs) and interactions with water for post-combustion carbon capture in a scientific and modeling effort to determine “New Materials and Process Development for Energy-Efficient Carbon Capture in the Presence of Water Vapor”. The experimental effort is informed by computational screening and process-level modeling. Early work favors fluorinated MOFs, because they selectively adsorb CO<sub>2</sub> in the presence of water vapor. The process-level modeling work indicates that it may be economically and technically feasible to remove water prior to carbon capture. However, the volume of water to be removed will be determined by the integration of materials development in future work.

Pre-combustion capture research balances the GCEP carbon capture portfolio with a team of chemical and biological engineers led by Joan Brennecke at the University of Notre Dame. They are researching “Chemically-Complexing Ionic Liquids for Pre-combustion CO<sub>2</sub> Capture”. They plan to design and develop ionic liquids (ILs) from pre-combustion in applications such as integrated gasification combined cycle systems. At the end of their three-year project, the

investigators hope to achieve 90% pre-combustion CO<sub>2</sub> capture with no greater than a 10% energy penalty and 15% increase in cost. In the first seven months of research, the team has performed quantum calculations of binding energies of candidate materials, synthesized three ILs that demonstrate structural cooperative complexation, and characterized and measured the CO<sub>2</sub> capacity of these materials.

Systems analysis work is being conducted in two separate programs by researchers at Stanford University and Carnegie Mellon University. At Stanford, Christopher Edwards and Adam Brandt are leading an effort on “Carbon Capture Systems Analysis: Comparing Exergy Efficiency and Cost of Electricity of Existing and Future Technology Options”. Their objective is to develop a framework based on an exergetic analysis at the local (system) and global (life cycle) level in addition to a techno-economic evaluation of capture technologies. Four types of CCS technologies are being studied under this framework: MEA/NGCC as a reference system, MOFs-based adsorption, biomimetic sorbents and ionic liquids absorption. To date, Matlab codes are being developed for both the systems level and life cycle assessment.

Edward Rubin is leading the systems analysis team at Carnegie Mellon University on “Systems Analysis of Advanced Power Plant Carbon Capture Technologies”. This work will expand on the existing Integrated Environmental Control Model (IECM) framework to allow for carbon capture technology evaluation. Work on the project did not begin until February 2013, initial progress has been to review literature, formulate process designs and thermodynamic models of the MOFs funded by GCEP for incorporation into IECM.