Introduction to CO_2 Capture

The generation of carbon dioxide is a direct consequence of extracting the maximum energy possible from fossil fuels. However, emissions of CO_2 to the atmosphere can be avoided by returning the carbon to the lithosphere. At sufficient purity, CO_2 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_2 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_2 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. Due to protracted contract negotiations, 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. The team has synthesized promising nitrogen-doped mesosporous carbons, and a thermogravimetric analysis method for monitoring the absorption/desorption kinetics has been developed.

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". Computational screening and process-level modeling inform the experimental effort. Through the computational screening method developed, fluorinated MOFs show promise of selectively adsorbing CO_2 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_2 Capture". They plan to design and develop ionic liquids (ILs) from pre-combustion is 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_2 capture with no greater than a 10% energy penalty and 15% increase in cost. To date the team has developed a thermodynamic and process model that identifies the ideal reaction enthalpies for an ionic liquid that exhibit cooperative binding and many of the compounds have been synthesized. A new route for CO_2 caputre by phosphonium ylide has been characterized. Also computational methods have been made to explain the physical cooperativity of CO_2 and mixed gases.

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. There has been much progress on the systems analysis and life cycle assessment efforts. There now exists a Matlab model to calculate the exergy of any gas-adsorbed phase used for carbon capture. This analysis fills a gap in adsorption gas separation systems and addresses the funded work on MOF and biomimetic sorbent systems. The life-cycle analysis is extracting information from the *Ecoinvent v.3* dataset using custom code to manipulate and return the flows of exergy for a preliminary analysis of NGCC and PCC power plants with and without amine-absorption carbon capture.

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. The team has assessed the available data on material properties of ionic liquids and MOFs and used the information to develop preliminary technical and economic MATLAB models.