

Carbon Mitigation

Objective

The goal of this project is to identify and develop standards and measurement methods currently needed by the energy industry to enable the development of cost efficient carbon mitigation technologies. The project aims to develop standard reference materials (SRM™) as well as construct a physico-chemical property/performance database for a variety of sorbent materials that will help industry define the specific properties that play a major role in CO₂ adsorption and regeneration. In addition, the project will address current measurement challenges in the evaluation of critical properties of membranes and sorbent materials.



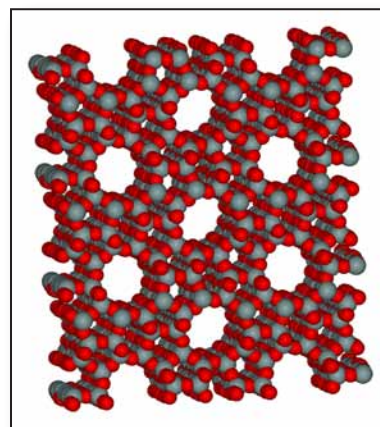
Impact and Customers

- The continual rise in anthropogenic atmospheric CO₂ and the concomitant effect on climate change underlie the urgent need for the implementation of carbon mitigation approaches to stabilize the CO₂ concentration while more sustainable energy technologies are developed.
- Given the existing availability, of and dependence on, fossil fuel resources worldwide (particularly coal), fossil fuel based energy sources are expected to remain the predominant source of energy in the foreseeable future. A key step in carbon mitigation involves the separation and capture of CO₂ at point sources such as coal fired power plants. The prospects for developing commercially viable carbon capture and sequestration (CCS) technologies depend upon the added cost of generating electricity with CCS.
- Carbon capture technologies are very costly, in great part due to the energy required to regenerate the solvents currently available to capture CO₂. Current DOE targets for viable post-combustion technologies are 90% capture efficiency, with an associated increase in electricity costs no greater than 35%.
- Opportunities to decrease capture costs could come from the development of energy efficient solid sorbents and membranes. The achievement of this goal could be greatly accelerated through the development of standards and advances in measurement science. Potential customers include the fuel, oil, chemical, and building industries, as well as CO₂ sorbent manufacturers, carbon capture plant builders, and fossil fueled power plants.



Approach

Identification of standards and measurements needed in the carbon capture industry, and the subsequent construction of a carbon mitigation road map, will be accomplished in collaboration with leaders in the field. Outreach activities such as workshops and seminars will be an integral part of the program. Materials considered as potential candidates for SRMs will be tested through a comprehensive evaluation process. A reference property and performance database of the physico-chemical characteristics of the sorbent materials and their CO₂ sorption performance will provide industry with reliable information for the rational design of sorbents and their processing methods. State-of-the-art analytical tools will be integrated, and measurement methods developed for determining properties that are currently difficult to obtain or verify. Some of the techniques under development will enable the determination of pore architecture and "closed" porosity, *in-situ* monitoring of the structural response on CO₂ sorption in the presence of competing gases, and identification and location of atomic adsorption sites and adsorbate species.



Accomplishments

Activities in the carbon mitigation project will address current needs for standards and measurements in the area of membranes and solid sorbents for CO₂ separation and capture applications. A new laboratory is being built for assessing the performance of CO₂ sorbent materials based on capacity, kinetics, thermodynamics, life cycle, and selectivity. Equipment will include a high pressure thermogravimetric analyzer (TGA) integrated with an evolved gas analyzer (EGA) and a high pressure differential scanning calorimeter. In addition, high sensitivity volumetric measurements will be made using a custom-built, computer-controlled Sieverts apparatus.



MSEL Sustainability Series

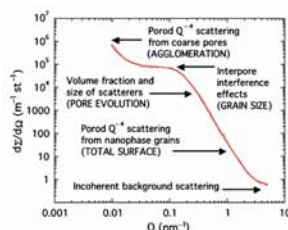
Working with government, industry and academic experts in carbon mitigation, MSEL researchers are identifying standards and measurement gaps in the area of CO₂ capture, to guide research and construct a CCS technology roadmap. This past year, MSEL organized a seminar series on sustainability that covered a variety of topics related to carbon mitigation. To this end, the carbon mitigation project is developing new tools and measurement methods motivated by three measurement challenges that have been identified: (1) characterization of pore architecture and “closed” porosity, (2) real-time monitoring of the structural response of sorbent materials on CO₂ sorption in the

presence of other gases commonly found in flue gas, and (3) *in-situ* identification and location of atomic adsorption sites and adsorbate species.



NIST Recommended Practice Guide SP-960-17

Proper characterization of sorbent materials with respect to specific surface area, porosity, pore size, and pore size distribution is important for ensuring the required performance. In recent years, NIST has participated in the development of a certified nanoporous reference material for mercury porosimetry (NIST SRM 1917/CRM BAM-P127) and also published a Recommended Practice Guide (jointly with the Federal Institute for Materials Research and Testing (BAM), in Germany) on “Porosity and Specific Surface Area Measurements for Solid Materials”.

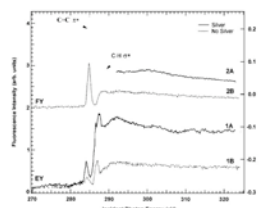


SANS data for a partially sintered nanoparticulate system

Evaluating changes in sorbent porosity after either surface functionalization or reaction with CO₂ is a challenge when using methods based on gas adsorption that can only

provide information about open porosity, and may be limited by diffusional hindrance of the gas used as a probe. MSEL expertise in the use of scattering techniques such as small angle neutron scattering (SANS) will enable a comprehensive picture of the structure that includes both open and closed porosity, pore surface characteristics, pore shape, pore size distribution and volume, spatial distribution, and pore network structure and morphology.

Changes in the crystalline structure of sorbent materials occurring during adsorption and desorption of CO₂ may play a very important role in the sorption mechanism. We are developing measurement methods to monitor lattice parameters and phase transformations via *in-situ* high pressure X-ray diffraction integrated with EGA, to complement high pressure TGA.



NEXAFS spectra of carbon-containing species adsorbed on LZ-52 faujasite

Another important aspect of the CO₂ sorption mechanism that will play a role in designing better sorbent materials involves the identification and location of adsorption sites, adsorbate species and reaction intermediates. Near edge soft X-ray absorption fine structure spectroscopy (NEXAFS), a nondestructive synchrotron based analytical tool, will be used for *in-situ* surface studies under different experimental conditions to probe the molecular bond chemistry, orientation, and concentration of the CO₂ adsorbed species, and reaction intermediates.

Learn More

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Publications

Klobes P, Meyer K and Munro RG *NIST Recommended Practice Guide on Porosity and Specific Surface Area Measurements for Solid Materials* (2006) http://www.nist.gov/public_affairs/practiceguides/SP960-17_RPG_Porosity1.pdf

Allen AJ, *Characterization of Ceramics by X-Ray and Neutron Small-Angle Scattering* J. Am. Ceram. Soc., 88: 1367 (2005)

Sambasivan S, Fischer DA, Kuperman A, and DeKoven BM *Direct Observation of Propylene Transformation Chemistry on and in the Pores of Silver Exchanged Faujasite Catalyst* Advanced Materials, 12: 1809 (2000)