Capture of CO_2 Project Fact Sheet List

Project Title	Primary Contractor	Fact Sheet Listing
OTM-Based OxyCombustion for CO_2 Capture from Coal Power Plants	Praxair, Inc.	C-3
CO_2 Hydrate Process for Gas Separation from a Shifted Synthesis Gas Stream	LANL/Nexant	C-5
Development of a Dry Sorbent-based Post-combustion Carbon Dioxide Capture Technology for Retrofit in Existing Power Plants	Research Triangle Institute	C-7
Thermally Optimized Membranes for Separation and Capture of CO_2	LANL & INEEL	C-9
CO_2 Capture for PC-Boiler Using Flue-gas Recirculation: Evaluation of CO_2 Capture/Utilization/Disposal Options	ANL	C-13
Carbon Dioxide Capture by Absorption with Potassium Carbonate	University of Texas at Austin	C-15
An Integrated Modeling Framework for Carbon Management Technologies	Carnegie Mellon University	C-17
Oxygen-Fired CO_2 Recycle for Application to Direct CO_2 Capture from Coal-Fired Power Plants	SRI International	C-21
Pilot-Scale Demonstration Of A Novel, Low-Cost Oxygen Supply Process And Its Integration With Oxy-Fuel Coal-Fired Boilers*	The BOC Group, Inc.	C-23
PC Oxycombustion Pilot Testing	Babcock & Wilcox	C-25
Ionic Liquids: Breakthrough Absorption Technology for Post-Combustion CO_2 Capture	University of Notre Dame	C-27
CO_2 Removal from Flue Gas Using Microporous Metal Organic Frameworks	UOP LLC	C-29
Biomimetic Membrane for CO_2 Capture From Flue Gas (SBIR)	Carbozyme,Inc.	C-31
Fabrication and Scale-up of Polybenzimidazole (PBI) Membranes for Pre-Combustion-Based Capture of Carbon Dioxide	SRI International	C-33
Development of Biomimetic Membrane for Near Zero PC Power Plant Emissions	Carbozyme,Inc	C-37

NETL Office of Research and Development Project Titles	Fact Sheet Listing
Modular CO_2 Capture Facility - CO_2 Capture Design Studies	C-39
Ammonia-Based Process for Multi-component Removal from Flue Gas	C-41
Solid Sorbents for CO_2 Capture from Pre Combustion Gas Streams	C-43
Mechanistic Study of CO_2 Adsorption on Solid Amine Sorbent	C-45
Molecular Design of CO_2 Ligands Ionic Liquids and Poly (Ionic Liquids)	C-47
Electrochemical Separation of CO_2	C-49
Solid Sorbents for CO_2 Capture from Powerplant Exhaust Streams	C-51
Reactor Design for CO_2 Capture Using Sorbents	C-53
Novel CO_2 - Philic Absorbents	C-55
Surface Immobilization Nanotechnology for CO_2 Capture	C-57
Development of Metal Organic Framework Materials for CO_2 Separation	C-59
Oxy-Fuel combustion	C-61
Chemical Looping for Combustion and Hydrogen Production	C-63

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

OTM-BASED OXYCOMBUSTION FOR CO_2 CAPTURE FROM COAL POWER PLANTS

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Background

Oxycombustion, or burning fuel in oxygen to generate flue gas consisting of primarily CO_2 and H_2O, is established as a credible means to facilitate CO_2 capture from coal power plants. The economics of conventional oxycombustion processes are currently limited by the parasitic power that is required for cryogenic oxygen production in conventional air separation units (ASU). A further limitation of oxycombustion is the requirement that a portion of the CO_2 in the exhaust must be cooled and recycled in order to maintain the temperature in the combustion chamber within practical limits. Praxair has developed novel OTM technology that has the potential to solve both of these issues. OTMs can be integrated such that there is minimal need for air compression and the parasitic power consumption required for oxygen production is reduced by 70-80% as compared to cryogenic ASU.

Under a prior agreement with the DOE, Praxair determined that the cost of CO_2 avoided from advanced boilers that use the integration of air separation from OTMs and oxyfuel combustion is competitive with other CO_2 capture processes when applied to large power plants. This work also demonstrated that durable oxygen transport membranes for oxyfuel combustion can be fabricated to survive and maintain reliability in a fuel environment. During the prior testing Praxair observed a zero percent failure rate for the OTM membranes being tested. However, the highly durable materials selected for the OTM reactors will require substantial development in order to improve oxygen flux through the OTM system, while maintaining durability, and reducing manufacturing costs.

Description

The basic principle behind the OTM oxycombustion system is the use of chemical potential for the oxygen separation driving force instead of pressure. In conceptual designs, the OTM is integrated directly with the boiler. The combustion reaction on the fuel side of the membrane creates a very low oxygen partial pressure compared to the air side of the membrane. This chemical potential difference drives oxygen through the membrane without the need for additional air compression.

PARTNERS

Praxair, Inc.
University of Utah

COST

Total Project Value
$8,358,445

DOE/Non-DOE Share
$5,432,989 / $2,925,456

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Objectives

Phase I Objectives:

- Increase oxygen flux of OTMs to commercial targets while maintaining the current levels of strength and reliability.
- Develop and down-select an optimum process integration cycle for OTM coal- based power system with CO_2 capture.
- Test the effects of coal and flue gas impurities on the performance of OTMs.

Phase II Objectives:

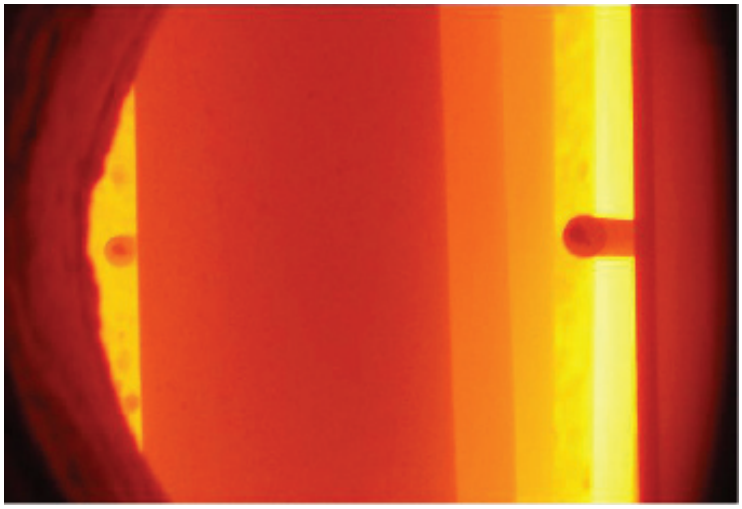
- Demonstrate ability to produce OTM tubes with appropriate dimensions and manufacturing yield required to proceed with pilot demonstration.
- Deliver preliminary engineering design for OTM pilot plant system.

Benefits

An OTM-based coal fired power process will help attain the Carbon Sequestration program goals by providing a highly concentrated, sequestration-ready stream of CO_2 without costly separation and cryogenic oxygen production.

Planned Activities

- Design, construct, and operate bench-scale OTM-coal reactor at the University of Utah for the evaluation of OTM performance in a coal-based power system.
- Conduct OTM manufacturing process development at Praxair OTM pilot manufacturing facility in Indianapolis, IA.
- Evaluate OTM performance improvements in single and multi-tube OTM reactors at Praxair research facilities in Tonawanda, NY.



OTM tubes during combustion testing in multi-tube reactor.

Project470.indd

PROJECT facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Sequestration and Gasification Technologies

04/2008

Carbon Dioxide Hydrate Process for Gas Separation from a Shifted Synthesis Gas Stream

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Background

One approach to de-carbonizing coal is to gasify it to form fuel gas consisting predominately of carbon monoxide and hydrogen. This fuel gas is sent to a shift conversion reactor where carbon monoxide reacts with steam to produce carbon dioxide (CO_2) and hydrogen. After scrubbing the CO_2 from the fuel, a stream of almost pure hydrogen stream remains, which can be burned in a gas turbine or used to power a fuel cell with essentially zero emissions. However, for this approach to be practical, it will require an economical means of separating CO_2 from mixed gas streams. Since viable options for sequestration or reuse of CO_2 are projected to involve transport through pipelines and/or direct injection of high pressure CO_2 into various repositories, a process that can separate CO_2 at high pressures and minimize recompression costs will offer distinct advantages. This project addresses the issue of CO_2 separation from shifted synthesis gas at elevated pressures.

The project is concerned with development of the low temperature SIMTECHE process, which utilizes the formation of CO_2 hydrates to remove CO_2 from a gas stream. Many people are familiar with methane hydrates but are unaware that, under the proper conditions, CO_2 forms similar hydrates. In Phase 1, a conceptual process flow scheme was developed. The thermodynamic limits of such a process were confirmed by equilibrium hydrate formation experiments for shifted synthesis gas compositions, and rapid hydrate formation kinetics were demonstrated in a bench-scale flow apparatus. Performance projections were then made for a few selected process configurations, and encouraging preliminary economics were developed.

Primary Project Goal

The goal of this project is to construct and operate a laboratory-scale unit utilizing the hydrate process for CO_2 separation.

Objectives

This project will investigate an innovative, proprietary, CO_2 capture technology that can be applied to integrated gasification combined cycle power plants and other industrial gasification facilities. The SIMTECHE CO_2-Hydrate Separation Process holds promise of not only greatly reducing CO_2 emissions but also reducing the costs and the energy penalty associated with the capture process.

PARTNERS

Nexant

Los Alamos National Laboratory

SIMTECHE

COST

Total Project Value
$14,385,000

DOE/Non-DOE Share
$5,435,000 / $0

Los Alamos National Laboratory DOE/Non-DOE Share
$8,950,000 / $0

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Objectives include:

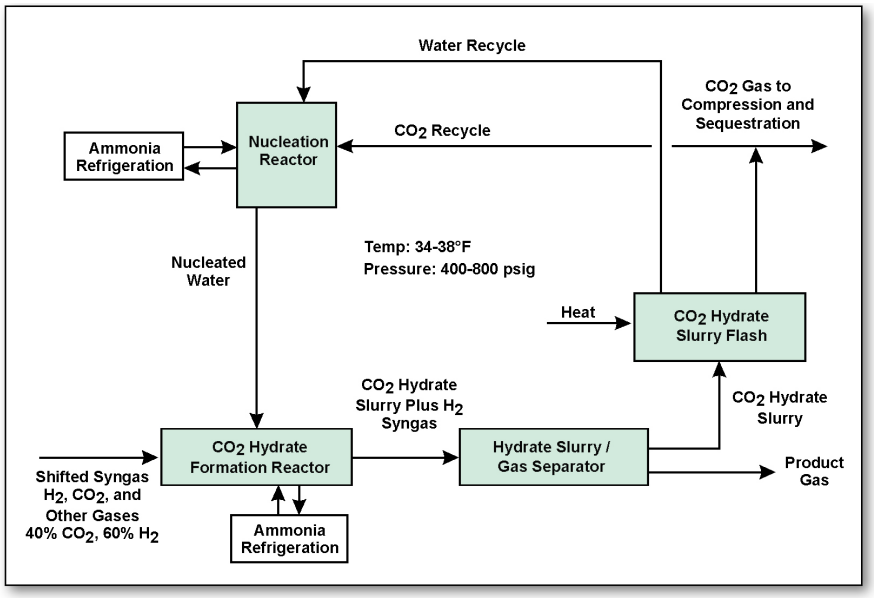
- Experimental confirmation of the feasibility of the proposed CO_2 hydrate concept.
- Extending previously developed process modeling to the latest proposed concept for the SIMTECHE process.
- Determining the ultimate reduction in CO_2 concentration that can be achieved and assessing the potential negative influence of H_2S and CH_4 on the process.
- Providing detailed design and operating data in preparation for field testing of a slipstream test unit at an industrial site.
- Assessing the impact of the experimental findings on the overall process economics and identifying critical properties and critical parameters.

Accomplishments

- Demonstrated the viability of low-temperature CO_2 separation from a mixed-gas stream through the formation of CO_2 hydrates.
- Potential 68 percent CO_2 removal was demonstrated during once-through operation at 1000 psi without promoters.
- Potential 90 percent CO_2 removal was demonstrated with promoters.
- Confirmed design residence time assumptions on both a kinetic and heat transfer basis.
- Engineering analysis showed that a two-stage Simteche process with a promoter and 90 percent CO_2 removal was most economic, and compared favorably with a two-stage Selexol process.

Benefits

The hydrate process will provide a high-pressure, low-temperature system for separating CO_2 from shifted synthesis gas in an economical manner. The process can be adapted to an existing gasification power plant for CO_2 separation in the production of synthesis gas. Overall, the process will result in a residual concentrated stream of hydrogen capable of fueling zero-emission power plants of the future and a concentrated CO_2 stream available for re-use or sequestration.



Project196.indd

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

04/2008

DEVELOPMENT OF A DRY SORBENT-BASED POST COMBUSTION CO_2 CAPTURE TECHNOLOGY FOR RETROFIT IN EXISTING POWER PLANTS

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Background

Currently available commercial processes to remove carbon dioxide (CO_2) from flue gas streams are costly and energy intensive. RTI International is heading a research team to continue development and scale-up of an innovative process for CO_2 capture that has significant potential to be less expensive and less energy intensive than conventional technologies. The "Dry Carbonate Process" utilizes a dry, regenerable, carbonate-based sorbent that captures CO_2 in the presence of water to form bicarbonate. Upon heating, the bicarbonate decomposes into a CO_2/steam mixture that can be converted to a pure CO_2 gas stream suitable for industrial use or sequestration. This process is ideally suited for retrofit in existing coal-fired power plants. With process modifications, it is anticipated the technology can also be used for CO_2 control from natural gas plants, cement plants, and refineries.

Description

To achieve the objectives of this project, RTI will continue research and development (R&D) work performed under a previous cooperative agreement with the U.S. Department of Energy's (DOE) National Energy Technology Laboratory (NETL). The project will be initiated by conducting technical and economic evaluations of various configurations of the Dry Carbonate Process. A down-selection process will be performed to identify the most promising process configuration. The project team will then fabricate and test process components at bench scale to confirm the feasibility of the selected process design. Following successful bench-scale testing, RTI and team members will design and fabricate a skid-mounted validation unit capable of capturing at least one ton of CO_2 per day. This unit will be fully commissioned at RTI. The unit will then be moved to the U.S. Environmental Protection Agency's (EPA's) site in Research Triangle Park, NC, where it will be tested extensively for one year with a slipstream of flue gas from the EPA's coal-fired combustion unit. Using data collected from this testing, the project team will optimize the process design and perform an economic evaluation for a commercial embodiment of the process. These results will be used to develop both a process package for a larger slipstream test unit (STU) and a detailed technology commercialization plan intended to attract utility company interest.

Primary Project Goal

The overall objective of this project is to perform the necessary research to scale up and test a commercially viable CO_2 capture process based on the reaction of

PARTNERS

RTI International

(RTI International is the trade name of Research Triangle Institute)

BOC Gases

EPRI / Nexant

ADA-ES

ARCADIS

PERFORMANCE PERIOD

03/07/2007 to 03/06/2010

COST

Total Project Value

$4,020,100

DOE/Non-DOE Share

$3,217,056 / $803,044

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sodium carbonate with CO_2 and water vapor present in the flue gas from a coal-fired combustion system.

Objectives

In addition to the overall objective, specific project objectives include:

- Demonstrating the operational feasibility of all process components.
- Demonstrating the process capacity to remove >90 percent of the CO_2 from flue gas.
- Demonstrating the sustained chemical and mechanical stability of the carbonate-based sorbent during testing.
- Demonstrating the process capacity to produce a pure CO_2 by-product stream.
- Demonstrating (through detailed analyses) the economic feasibility of the Dry Carbonate Process and the capability to meet DOE/NETL's economic benchmarks.

Benefits

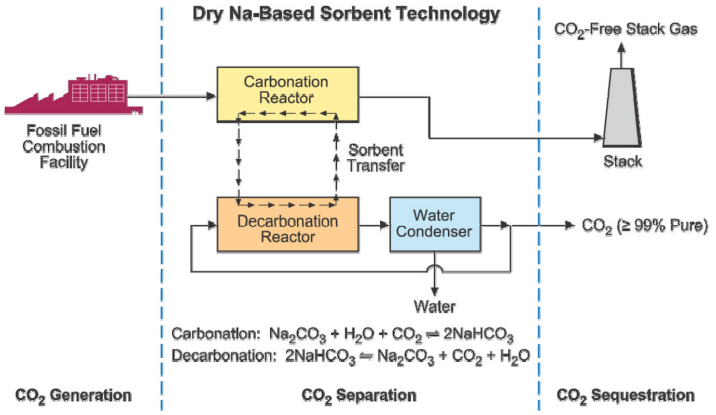
This technology will provide conventional coal-fired power plants, natural gas-fired plants, and advanced power generation systems with a less costly and less energy intensive process for removing CO_2 from flue gas.

Accomplishments

RTI and project team members have selected several process configurations that are currently being evaluated through technical and economic analyses. Several novel designs are being considered that are expected to address many of the process challenges associated with the Dry Carbonate Process. RTI is currently conducting laboratory testing to support theoretical calculations showing that significant improvements for heat control, heat transfer, sorbent inventory, and CO_2 removal capacity are possible with these new process designs.

Planned Activities

Additional bench-scale testing of various process components will be carried out following successful completion of the technical and economic evaluations mentioned above. The project team will put together a process design report for DOE/NETL review.



Project474.indd

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

4/2008

THERMALLY OPTIMIZED MEMBRANES FOR SEPARATION AND CAPTURE OF CARBON DIOXIDE

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Background

An important component of the DOE Carbon Sequestration Program is to develop carbon capture technologies for power systems. Capturing carbon dioxide (CO_2) from mixed-gas streams is a first and critical step in carbon sequestration. To be technically and economically viable, a successful separation method must be applicable to industrially relevant gas streams at realistic temperatures and volumes. The effectiveness of current technologies for separating CO_2 is limited. Amine-based technologies work only at low temperatures and pressure-swing absorption and cryogenic distillation have significant energy penalties (up to 35 percent) for separating CO_2. Polymer-based membrane separations are less energy intensive, requiring no phase change in the process, have been used successfully in a number of industrial applications, and typically provide low-maintenance operations. Successful synthesis gas separation using a polymer membrane requires a membrane that is thermally, chemically, and mechanically stable at high temperature and high pressure. Commercially available polymeric materials currently employed are not stable in such demanding environments. In general, as the glass transition temperature of the polymer is approached, membrane selectivity is significantly reduced and flux decline due to membrane compaction (creep) becomes more significant. In addition, current membrane materials are often subject to chemical degradation by the process stream, a problem that is exacerbated by elevated temperature.

Primary Project Goal

The overall goal of this project is to develop thermally, chemically, and mechanically stable polymeric-metallic composite membranes that can provide

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PARTNERS

Los Alamos National Laboratory

Pall Corporation

Idaho National Laboratory

University of Colorado

effective precombustion CO_2 capture under a broad range of conditions relevant to the power industry while meeting the Carbon Sequestration Program goals of 90 percent CO_2 capture at less than a 10 percent increase in the cost of energy services.

Objectives

The primary objective of this project was the development of innovative polymeric-metallic composite membrane structures (Figure 1) that achieve the critical combination of high selectivity, high permeability, chemical stability, and mechanical stability all at elevated temperatures (>150 °C). The research team pursued two major pathways to its primary goal. The first involved extending the current PBI-based polymeric-metallic composite membrane to its limits. The second pathway built upon the base PBI framework to develop materials with enhanced gas separation properties (primarily H2/CO_2 selectivity and H_2 flux) while maintaining the desirable chemical, mechanical, and thermal stability exhibited by the unmodified PBI and improving polymer solvent solubility.

Benefits

The base performance of the polymeric-metallic composite membrane structure has been determined from room temperature to 400 °C. The polymer maintains a commercially attractive selectivity between hydrogen (H_2) and CO_2 even at 400 °C (Figure 2). The PBI-based composite membrane outperforms any polymer-based membrane available commercially or reported in the literature for separations involving hydrogen. This achievement is validated via membrane productivity (separation factor and flux) comparisons. Additionally, the improved performance of this technology in an application such as integrated gasification combined cycle-integrated capture is further substantiated by the accessible operating temperature range and the chemical stability of the composite membrane in challenging operating environments.

Accomplishments

- Fabrication and testing of the first polybenzimidazole (PBI)-based composite polymeric-metallic membrane structure (in flat disk and tubular formats) that is selective from room temperature to >400 °C than current commercially available polymeric membranes (<150 ˚C). This achievement represents the highest demonstrated operating temperature at which a polymer-based membrane has successfully functioned.

- Improvements to the intermediate layer on the outside diameter of Pall's AccuSep® tubes resulting in a smooth, high porosity, defect-free surface.

- Successful long-term testing of the polymeric-metallic composite membrane in dry gas environments containing H_2, CO_2, methane (CH_4), nitrogen (N_2), carbon monoxide (CO), and hydrogen sulfide (H_2S) from 25 - 400 °C. Demonstration of the membrane's thermal stability via 300+ days in operation at 250 °C.

- Successful out-of-the-laboratory slip-stream testing of the polymeric-metallic composite membrane on a natural gas fuel processor. The test stream consisted of the fully hydrated natural gas reformate exiting the water gas shift reactor. Testing was conducted from 250 - 400 °C.

- Development and demonstration of an innovative methodology that enables the simultaneous measurements of gas permeation and membrane creep at elevated temperatures. This technique provides a unique approach to the optimization of long-term membrane performance under challenging operating conditions and has been utilized to obtain the first-ever transport-mechanical property dataset for PBI at elevated temperatures.

- Synthesis of a number of new PBI-based compounds by post-polymerization modification.

- Demonstration of commercialization potential.

PERFORMANCE PERIOD

05/15/2000 to 09/30/2006

COST

Total Project Value
$5,118,000

DOE/Non-DOE Share
$3,998,000 / $1,120,000

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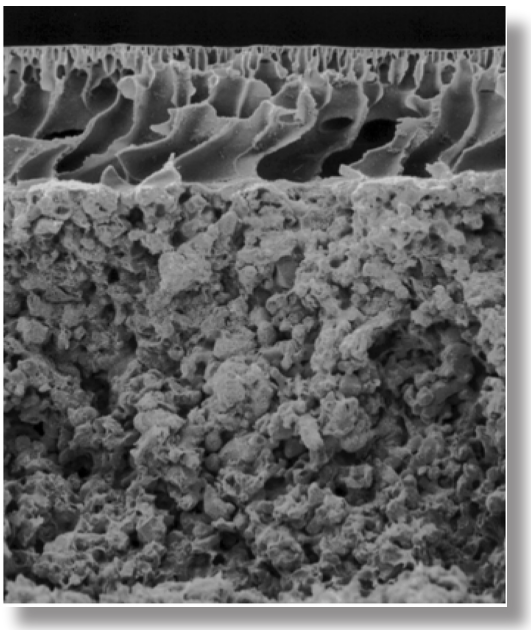

Figure 1. Scanning electron microscopy image of a poly-benzimidazole (PBI)-based polymeric-metallic composite membrane cross-section. The polymeric selective layer is the thin skin at the surface of the composite structure.

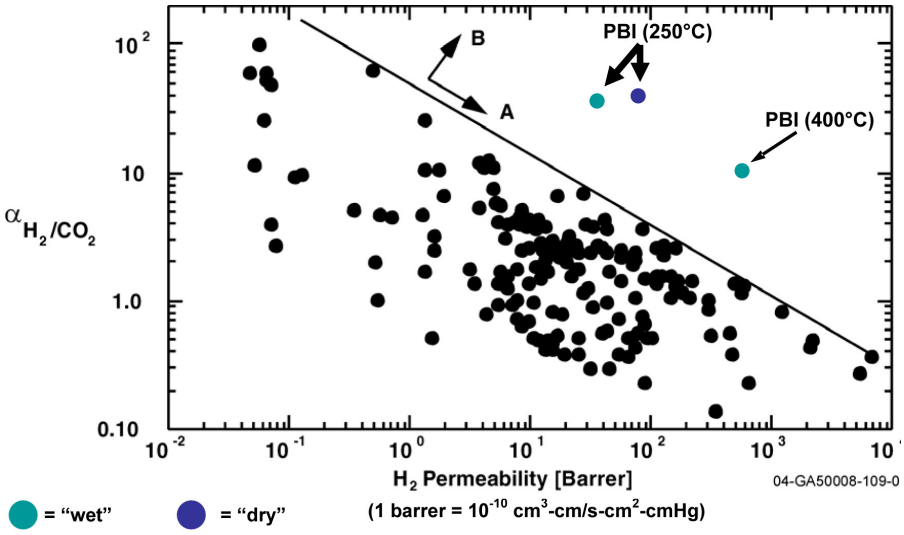

Figure 2. Trade-off plot between H_2 permeability and H_2/CO_2 selectivity in polymers. The data points for PBI reflect measurements made at high temperature. Note the excellent combination of permeability and selectivity.

Project194.indd

PROJECT facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Carbon Sequestration

04/2008

Evaluation of Carbon Dioxide Capture/Utilization/Disposal Options

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Background

Concerns over possible global climate changes due to increasing atmospheric concentrations of greenhouse gases such as carbon dioxide (CO_2), have placed a strong emphasis on the development of high-efficiency, coal-based energy systems, as well as on processes for recovering and sequestering CO_2 that is produced. One approach is oxycombustion with flue gas recycle to maintain a normal temperature profile in the furnace. Oxycombustion with flue gas recycle is an emerging technology that has the potential to allow for control of CO_2 emissions at a lower cost than a conventional air-fired pulverized coal (PC) power plant.

Description

The U.S. Department of Energy is investigating the feasibility of retrofitting boilers using this concept as a strategy for CO_2 recovery from conventional PC power plants. This approach was conceived nearly 20 years ago at Argonne National Laboratory (ANL) as a low-cost CO_2 source for enhanced oil recovery (EOR). A CO_2/oxygen (O_2) molar ratio of about three is necessary to preserve the heat-transfer performance and gas-path temperatures, allowing this system to be applied as a retrofit.

The principal contribution of this project is to develop engineering evaluations for the capture and recovery of CO_2 from PC-fired power plants that are retrofitted for flue gas recirculation. The full energy cycle will be considered, including mining, coal transportation and preparation, the PC-fired boiler with power generation, particulate removal and flue gas recirculation, facility water use, pipeline CO_2 conditioning, and CO_2 pipeline transport. ANL will also identify existing power plants that may be retrofit candidates, and will consider the effects of different coals on CO_2 capture as well as on the accessibility of sequestration options. In addition, the cost of retrofitting the existing fleet of domestic PC boilers with oxycombustion will be assessed by incorporating the AMIGA (All-Modular Industry Growth Assessment) macroeconomic model.

The project will provide the U.S. power industry with a low-cost retrofit system that could remain in service during future upgrades at power plants. The captured CO_2 can be used for EOR or otherwise sequestered. In general, the project addresses both design and full energy-cycle issues pertaining to existing coal-fired power plants.

PARTNERS

Argonne National Laboratory

PERIOD OF PERFORMANCE

10/01/1997 to 12/31/2010

COST

Total Project Value

$2,464,000

DOE/Non-DOE Share

$2,464,000 / $0

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Primary Project Goal

The goal of the project is to conduct comparative engineering assessments of technologies for the recovery, transportation, and utilization/disposal of CO_2 produced in high-efficiency, coal-based, energy systems. Coordinated evaluations will address CO_2 transportation, CO_2 use, and options for long-term sequestration. Commercially-available CO_2 capture technologies will provide performance and economic baselines for comparing innovative CO_2 recovery technologies across the full energy cycle.

Objectives

- Develop engineering evaluations for the recovery of CO_2 from PC-fired power plants retrofitted for flue gas recirculation and reconcile and extend these studies across the full energy-cycle.
- Identify existing power plants that may be retrofit candidates, considering the effects of different coals and the accessibility of a sequestration zone.
- Conduct analyses of an oxycombustion retrofit at large PC-fired power plants with AMIGA, regarding least-cost investment and ranking, as well as dispatch order and energy use in the economy.

Benefits

PC plants are the most common type of power plant; therefore, a system that can be retrofitted to PC-fired boilers and enable CO_2 recovery will have broad applicability. Flue gas recirculation eliminates the need for nitrogen (N_2)/CO_2 separation and sulfur separation, permitting more economical CO_2 recovery than competing amine-based systems. Technical and economic analyses will build on current accomplishments to develop a lower cost CO_2 capture technology.

Accomplishments

- A full energy cycle was evaluated based on simulation of an O_2-blown PC boiler with CO_2 recovery and flue gas recirculation that includes details of stream compositions for the whole system.
- Process design and economics for 300–900 MW PC-fired boilers burning low-, medium-, and high-sulfur coals have shown that oxycombustion is economical and could be an approach to lower the costs of eventually repowering a site with an integrated gasification combined cycle (IGCC) system.
- A draft report discussing the economics of oxycombustion and flue gas recirculation for low-, medium-, and high-sulfur coals was completed.
- A CO_2 pipeline network for the PJM region was postulated so that logistics and costs of CO_2 transport from oxycombustion power plants could be scoped out on a regional basis. This effort was then extended to the Illinois Basin, examining the logistics for an oxycombustion retrofit at a specific power plant on the edge of the Illinois Basin.
- Updated models to better define the performance and impacts of a high CO_2, low N2 flue gas.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

04/2008

CARBON DIOXIDE CAPTURE BY ABSORPTION WITH POTASSIUM CARBONATE

Background

Although alkanolamine solvents, such as monoethanolamine (MEA) and solvent blends have been developed as commercially-viable options for the absorption of carbon dioxide (CO_2) from waste gases, natural gas, and hydrogen streams, further process improvements are required to cost-effectively capture CO_2 from power plant flue gas. The promotion of potassium carbonate (K_2CO_3) with amines appears to be a particularly effective way to improve overall solvent performance. K_2CO_3 in solution with catalytic amounts of piperazine (PZ) has been shown to exhibit a fast absorption rate, comparable to 30 wt% MEA. Equilibrium characteristics are also favorable, and the heat of absorption (10-15 kcal/mol CO_2) is significantly lower than that for aqueous amine systems. Studies also indicate that PZ has a significant rate of reaction advantage over other amines as additives.

Description

The University of Texas at Austin will investigate an improved process for CO_2 capture by alkanolamine absorption/stripping that uses an alternative solvent, aqueous K_2CO_3 promoted by PZ. If successful, this process would use less energy for CO_2 capture than the conventional MEA scrubbing process. An improved capture system would mean a relative improvement in overall plant efficiency.

The project will include the development of models to predict performance of absorption/stripping of CO_2 using the improved solvent and performing a pilot plant (see figure) study to validate the process models and to define the range of feasible process operations. As part of the pilot plant study, a test with MEA will be conducted as a baseline to compare CO_2 absorption and stripping performance with tests using the K_2CO_3/PZ solvent. Researchers will also investigate key issues such as solvent degradation, solvent reclamation, and corrosion as well as alternative stripper configurations.

Pilot Plant at the University of Texas

Primary Project Goal

The primary goal of this work is to improve the process for CO_2 capture by alkanolamine absorption/stripping by developing an alternative solvent, aqueous K_2CO_3 promoted by PZ.

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PARTNER

University of Texas at Austin

PROJECT DURATION

07/09/2002 to 08/31/2007

COST

Total Project Value
$2,262,325

DOE/Non-DOE Share
$1,565,275 / $697,050

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Objectives

- To improve the process for CO_2 capture by developing aqueous K_2CO_3 promoted by PZ as an alternative solvent to MEA.
- To develop a system model based on data from bench-scale operations.
- To perform pilot-scale experiments to validate the process model and define the range of feasible process operations.
- To optimize process variables, such as operating temperature, solvent rate, stripper pressure, and other parameters.
- To quantify the effectiveness of the promoter.

Benefits

The major benefit of this project would be the ability to decrease the energy requirement for CO_2 capture from fuel gas or flue gas streams. Should CO_2 capture and sequestration become necessary, an improved capture process would significantly improve overall plant efficiency. The capital and operating costs for CO_2 capture could also be reduced.

Accomplishments

- Three solvents (7 molal (m) MEA, 5 m K_2CO_3/2.5 m PZ, and 6.4 m K_2CO_3/1.6 m PZ) were evaluated in four pilot-scale testing campaigns with three different absorber packings (two structured and one random).
  - To achieve equivalent absorber performance, 5 m K_2CO_3/2.5 m PZ requires two times less packing than 7 m MEA and three times less packing than 6.4 m K_2CO_3/1.6 m PZ.
  - The effective wetted area of two structured packings, Flexipak AQ Style 20 (213 m^2/m^3 dry area) and Flexipak 1Y (410 m^2/m^3), is 50 to 60 percent and 80 percent of that measured by CO_2 absorption from air by 0.1 N and NaOH, respectively.
- A rate-based model of absorber performance was developed in AspenPlus® with the RateSep™ block. This model was used to interpret pilot plant data and to predict performance at design conditions with and without intercooling.
  - The effective working capacity of 4 m K_2CO_3/4 m PZ is about 60 percent greater than 7 m MEA, and the heats of absorption are nearly equivalent.
  - The rate of CO_2 absorption in 4 m K_2CO_3/4 m PZ is 20 to 50 percent faster than in 7 m MEA.
  - Absorber intercooling is effective at enhancing system performance when the temperature bulge is in the middle or lower end of the column, at moderate liquid-to-gas ratios, and typically with higher capacity solvents.
- Three stripper models were developed: one in Aspen Custom Modeler (ACM) based on equilibrium stages, a rate-based model in ACM, and an equilibrium model in AspenPlus®. These models were used to estimate and compare energy requirements of alternative solvents and process configurations.
  - The double matrix stripper configuration is effective and produces some of the CO_2 at higher pressure.
- Studies of solvent loss, degradation, and reclamation have been completed.
  - PZ loaded with CO_2 shows less than 3 percent loss of PZ when heated at 135 °C for 8 weeks, compared to 60 percent loss of 11 m MEA at the same conditions.
  - The rate of oxidative degradation for PZ is low in the absence of dissolved copper.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

4/2008

AN INTEGRATED MODELING FRAMEWORK FOR CARBON CAPTURE AND STORAGE TECHNOLOGIES

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Background

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory (NETL) is developing safe, lower-cost methods of carbon dioxide (CO_2) capture and storage (CCS) as a potential option for climate change mitigation. In addition to technology development, there is a need for modeling and assessment tools to evaluate and compare the cost and effectiveness of CCS methods. Analytical tools also are needed to help identify and prioritize the most promising research and development efforts. This project was initiated in July 2000 to develop and demonstrate such capabilities.

Integrated Environmental Control Model Framework

Carnegie Mellon University (CMU) has developed the Integrated Environmental Control Model (IECM) to provide electric utility companies, equipment suppliers, government agencies, researchers, and policy analysts with an easy-to-use tool for estimating the performance, emissions, and cost of alternative fossil fuel power plant configurations and emission control technology scenarios. In the current project, the IECM is being extended to incorporate current and advanced systems for CCS as model options in addition to control technology options for criteria air pollutants and air toxics such as sulfur dioxide (SO_2), nitrogen oxides (NOx), particulates, and mercury. Figure 1 shows a schematic of the model inputs, outputs, and internal structure.

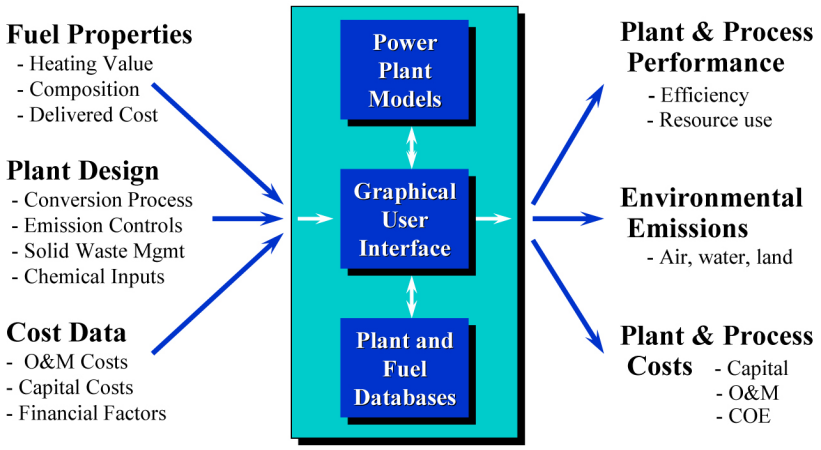

Figure 1. Structure of the IECM modeling environment. A graphical user interface allows the model to be easily used to configure a plant design of interest, set values for key parameters, and get results in tabular or graphical form.

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The power system options incorporated in the IECM include a pulverized coal-fired (PC) power plant, a natural gas-fired combined cycle (NGCC) power plant, and a coal-based integrated gasification combined cycle (IGCC) plant. Input parameters for all three systems can be adjusted to represent either current technology or advanced, high-performance designs. The IECM thus can be used to simulate advanced gasification-based as well as advanced combustion-based designs for power systems with near-zero emissions. In all cases, the probabilistic capability of the IECM allows uncertainties in performance and cost results to be quantified, enabling more rigorous assessments of technological risks and benefits.

Options for CO_2 Capture, Transport, and Storage

The IECM incorporates a variety of CCS options for both pre-combustion and post-combustion CO_2 capture, as well as oxyfuel combustion for PC plants. To simulate a complete CCS system, the costs of CO_2 transport and storage also are included in the modeling framework. Figure 2 shows a schematic of the overall system.

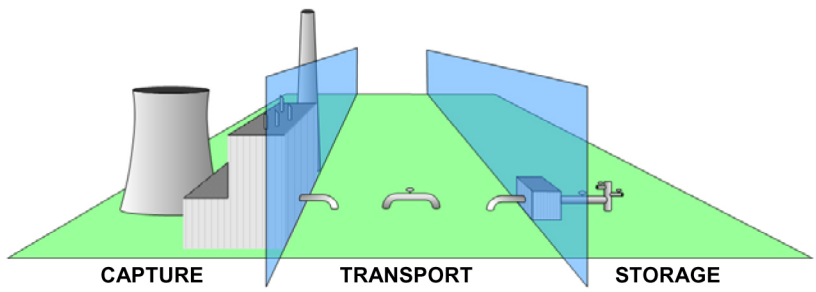

Figure 2. The IECM framework includes component modules and options for CO_2 capture, transport, and storage. CO_2 compression is included as part of the capture system.

CO_2 capture process options incorporated in the IECM include an amine-based chemical absorption system for post-combustion capture on PC and NGCC plants and a sorbent-based physical absorption system for pre-combustion capture at IGCC plants. The oxyfuel plant option produces a concentrated CO_2 stream using oxygen rather than air for combustion in a PC plant, with recycle of the CO_2-rich flue gas. Additional options under development include advanced power system components and CO_2 capture technologies promising lower costs.

The IECM also includes a CO_2 pipeline transport model plus several options for CO_2 storage, including geological sequestration in deep saline formations, in depleted oil reservoirs using enhanced oil recovery (EOR), or in unmineable coal seams with enhanced coal bed methane recovery (ECBM). An option for ocean sequestration also is available. For all plant designs, interactions between the CCS system and other environmental control technologies is accounted for in simulations of overall plant performance, emissions, and cost. Figure 3 illustrates several of the input and output screens available in the IECM.

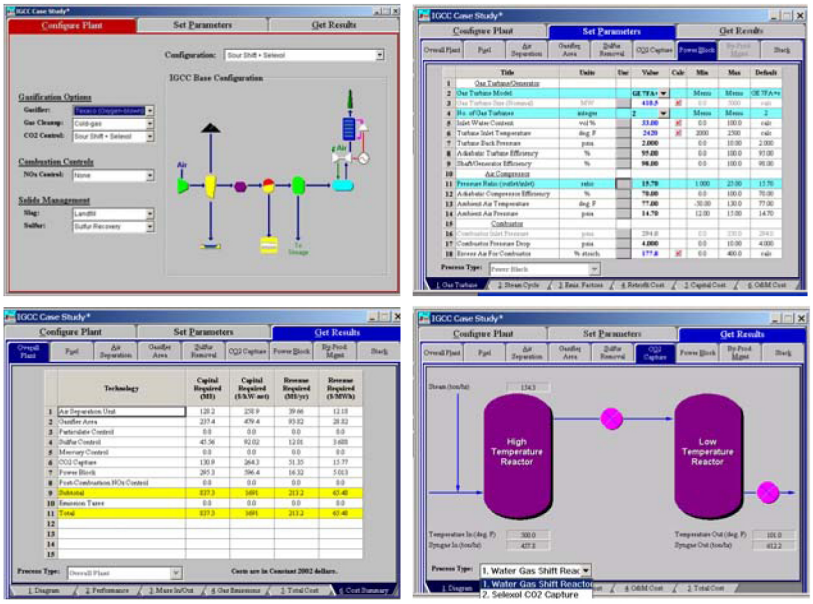

Figure 3. Sample screens from the IECM graphical user interface for a case study of an IGCC plant with CCS. Tabs at the top and bottom of each screen allow a user to configure the plant, set values of key design parameters, then get results for the overall plant or a specific component, such as the water gas shift reactor illustrated in the lower right

Benefits

The IECM—

- Determines the economic cost and cost of CO_2 avoided for alternative plant designs.
- Identifies the most cost-effective CCS options for a particular application.
- Simulates and optimizes the environmental design of new or existing power plants.
- Quantifies plant resource requirements and multimedia environmental emissions.
- Characterizes impacts of key interactions between plant components.
- Has fast run-time on a desktop or laptop computer, which provides reliable results without costly setup time or waiting.
- Quantifies the benefits of R&D, and identifies options with the highest potential payoffs.

- Is fully supported, documented, and updated periodically.

- Is available free online at www.iecm-online.com.

Accomplishments

- Developed and demonstrated a flexible modeling framework for the preliminary design of power plants employing CO_2 capture and storage.

- Provided a tool that can be freely and widely used to simulate and analyze alternative power systems and emission control options.

- Accounted for avoided carbon emissions, as well as multi-pollutant impacts for criteria air pollutants, air toxics and solid wastes.

- Estimated the costs of plant components and the overall system and its dependence on key design, operating, and financial parameters.

- Accounted for uncertainties in model input parameters and their influence on results.

- Made available free online at www.iecm-online.com

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Project279.indd

PROJECT facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Carbon Sequestration

04/2008

Oxygen-Fired CO_2 Recycle for Application to Direct CO_2 Capture from Coal-Fired Power Plants

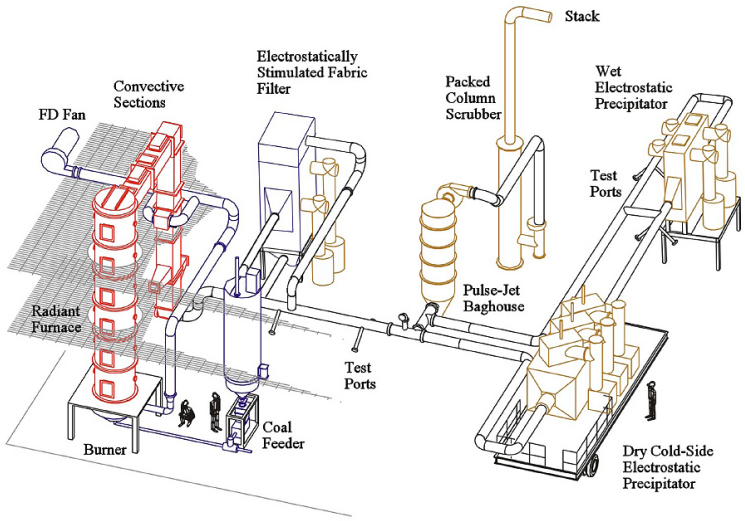
Background

Concern continues to mount over greenhouse gas emissions and their role in global climate change; and, if we are to continue burning coal, our most abundant fossil fuel, it is necessary to develop coal combustion technologies that can limit carbon dioxide (CO_2) emissions to the atmosphere. Oxycombustion is an emerging technology that has the potential to allow for control of CO_2 emissions at a lower cost than a conventional air-fired pulverized-coal (PC) power plant.

Description

Oxycombustion involves replacing air with pure oxygen in a PC boiler. The use of oxygen results in a lower volume of flue gas with a much higher concentration of CO_2 (greater than 60 percent by volume). The CO_2 is separated from water vapor by condensing the water through cooling and compression. Further treatment of the flue gas may be needed to remove pollutants and non-condensed gases (such as nitrogen) prior to CO_2 storage.

However, the advantages of oxycombustion are offset, to some extent, by the cost of providing high-purity oxygen (95 to 99 percent assumed in most current designs). In addition, combusting coal in pure oxygen results in temperatures that are too high for existing boiler and turbine materials; therefore, part of the CO_2-rich flue gas



Schematic of the Southern Research/Southern Company Combustion Research Facility

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Southern Research Institute

BOC Gases

MAXON Corporation

Reaction Engineering International

DTE Energy

PERFORMANCE PERIOD

09/27/2005 to 09/26/2008

COST

Total Project Value
$1,079,654

DOE/Non-DOE Share
$863,723 / $215,931

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must be recycled to the boiler to reduce the temperature in retrofit applications. Through this project, Southern Research Institute will explore the feasibility of retrofitting existing PC plants with oxycombustion systems.

Primary Project Goal

The primary project goal is to thoroughly investigate, develop, optimize, and model oxycombustion and CO_2 recycle to assess its feasibility for retrofit to existing PC-fired power plants.

Objectives

- Modify the pilot-scale Combustion Research Facility (CRF) to allow oxygen-fired and CO_2-recycle operations.
- Collect data on furnace temperatures, unburned carbon, gas composition, and flow rates into and out of the furnace.
- Evaluate the effect of various parameters, including firing configuration, oxygen purity, CO_2 recycle rate, oxygen concentration, and coal type.
- Design, manufacture, and install an oxycombustion burner specifically for the CRF.

Benefits

A number of studies have shown that recovering CO_2 from the flue gas at a PC-fired boiler will significantly increase the cost of electricity (COE). The main reasons are that the volume of gas is very large and the concentration of CO_2 is low, typically less than 15 percent. Commercially available absorption processes, such as amine-based systems, require large vessels and consume considerable parasitic power. Development of oxycombustion will minimize the volume of flue gas produced and increase the CO_2 concentration, thereby significantly reducing CO_2 capture cost relative to commercially available CO_2 absorption processes. Retrofitting oxycombustion at existing PC power plants also will enable CO_2 capture goals to be met at a lower capital investment than would be required to construct new facilities.

Accomplishments

- The design of facility modifications and additions is complete.
- The oxygen pad site has been determined.
- Oxygen mixing and control systems have been developed.

Planned Activities

- Construction of the flue gas recycle loop is expected to begin in FY 2008.
- Conduct flue gas recycle, oxycombustion experiments on various coals in the CRF facility.
- Adjust the existing CRF computational fluid dynamics model to incorporate flue gas recycle and oxygen-firing.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

PILOT-SCALE DEMONSTRATION OF A NOVEL, LOW-COST OXYGEN SUPPLY PROCESS AND ITS INTEGRATION WITH OXY-FUEL COAL-FIRED BOILERS

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Background

It is widely accepted that global climate change is due, in large part, to the emissions of greenhouse gases such as CO_2. Since fossil fuels will remain the primary energy source for some time, coal-fired power plants of the future will need to incorporate processes that can cost-effectively capture and sequester their CO_2 emissions. One of the promising CO_2 capture technologies is oxy-combustion with flue gas recycle. In this process, the combustion air is replaced with a mixture of oxygen and recycled flue gas to produce a CO_2 - flue gas, which can be conditioned and delivered to a CO_2 sequestration site. Recycled flue gas moderates temperatures and maintains heat transfer characteristics in the boiler, enabling the technique to be easily applied to existing coal-fired power plants. However, the biggest barrier to implementation of this technology is the cost of producing the oxygen. The standard oxygen production method for applications of this scale is the relatively costly cryogenic air separation process. The development of cost effective alternative technologies for oxygen production is extremely important to make oxy-fuel coal fired power plants with CO_2 capture viable and attractive.

One alternative to cryogenic air separation being investigated by BOC is the Ceramic Autothermal Recovery (CAR) oxygen production process. BOC, the world's second largest industrial gas company, has developed a novel high-temperature sorption-based technology for oxygen production and supply to oxygen-fired boilers with flue gas recycle.

Description

The process utilizes the oxygen storage capacity of Perovskite materials at high temperatures, and involves cyclic operation with conventional fixed bed vessels that contain the material in granular form. This process consists of two main steps: (1) oxygen sorption and (2) oxygen release. In step 1, air is passed through one bed to allow sorption and storage of oxygen, while in Step 2, a sweep gas such as flue gas or steam is passed through the other bed to release the stored oxygen. The process operation is made continuous by operating two beds in a cyclic mode. The air and purge steps are carried out counter-currently in order to achieve higher oxygen concentrations in the product mixture as well as to effectively recover the heat in the gas streams leaving the bed. Since oxygen sorption on Perovskites is exothermic while oxygen release is endothermic, the process operates autothermally with little heat input.

PARTNERS

Alstom Power Plant Laboratories

Western Research Institute

COST

Total Project Value
$6,132,613

DOE/Non-DOE Share
$4,906,089 / $1,226,524

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Primary Project Goal

The overall goal of the project is to conduct pilot-scale testing of BOC's Ceramic Autothermal Recovery (CAR) oxygen generation process, when integrated with a coal-fired combustor to produce a CO_2 - rich flue gas. This includes integrated testing of a 0.7 ton oxygen per day unit at WRI and scale up to a 10 ton oxygen per day unit and integrated testing at Alstom.

Objectives

- Determine the ability of CAR materials to handle the contaminants in the recycled flue gas stream including SO_2, NO_x and particulates at the levels present after processing in the scrubber and barrier filters.
- Determine the ability of the CAR test unit to operate at performance levels indicated as acceptable according to a systems and economic analysis.
- Assess the performance of the CAR test unit through an updated process and economic systems analysis to determine the ability to achieve economic and DOE goals.

Accomplishments

- The 0.7 ton oxygen per day CAR unit was operated at the Combustion Test Facility (CTF) of the Western Research Institute (WRI) that demonstrated that researchers were able to maintain operation of the CAR unit at the desired operational temperature range. This was accomplished by switching the feed gas to the bed from air to carbon dioxide.
- Subsequent testing at WRI demonstrated the ability to operate the CAR unit in dual bed cyclic mode.
- Conducted preliminary evaluations of CAR performance in the presence of recycled flue gas contaminants.
- Completed baseline oxycombustion tests for the CTF facility.

Planned Activities

- Complete integration of CAR unit dual bed system with the CTF facility at WRI to conduct integrated oxycombustion testing.
- Design and construct 10 ton oxygen/day CAR unit
- Integrate 10 ton oxygen/day CAR unit with Alstom's Multi-use Test Facility (MTF) in Winsor, CT.
- Test integrated CAR-MTF system in both pulverized coal and circulating fluidized bed combustion configurations.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

DEVELOPMENT OF COST EFFECTIVE OXY-COMBUSTION TECHNOLOGY FOR RETROFITTING COAL-FIRED BOILERS

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Background

Electric power generation from fossil fuels represents one of the largest contributors to greenhouse gas emissions, not just in the United States, but throughout the world. Various technologies and concepts are being investigated as means to mitigate carbon dioxide (CO_2) emissions. The concept of pulverized coal (PC) oxy-combustion is one potential economical solution, whereby coal is combusted in an enriched oxygen environment using pure oxygen diluted with recycled flue gas. In this manner, the flue gas is composed primarily of CO_2 and H_2O, so that a concentrated stream of CO_2 is produced by simply condensing the water in the exhaust stream. An advantage of oxy-combustion over air-fired combustion is that it provides a high potential for a step-change reduction in both CO_2 separation and capture costs because virtually all of the exhaust effluents can be captured and sequestered (co-sequestration).

Description

This project entails pilot-scale develop-ment of oxy-combustion technology for both wall-fired and cyclone boiler configurations. For the wall-fired mode, tests will include lignite firing, while cyclone boiler combustion tests will investigate different coal ranks. Parametric and 100-hour continuous tests will optimize the oxy-combustion process and assess the slagging, fouling, heat transfer, and overall operability characteristics. Specifications for flue gas purification, compression, transportation, and sequestration will be developed to help design the environmental equipment required (e.g. scrubber, selective catalytic reduction (SCR), etc). An engineering feasibility and economic evaluation will also be performed on a full-size cyclone boiler and a full-size wall-fired boiler. An ASPEN model will be developed to optimize the integration of the air separation unit (ASU), flue gas purification, CO_2 compression train, CO_2 transportation, and sequestration. Net power production will be calculated and the cost of electric production will be estimated using an economic model.

Primary Project Goal

The primary project goal is to further develop the oxy-combustion technology for commercial retrofit in existing wall-fired and cyclone boilers by 2012. To meet this goal, a two-phase research project is proposed that includes pilot-scale testing and a full-scale engineering and economic analysis.

PARTNERS

Babcock & Wilcox Company

AirLiquide

Battelle

PROJECT DURATION

3/31/2006 to 3/31/2008

COST

Total Project Value
$3,453,287

DOE/Non-DOE Share
$2,762,643 / $690,644

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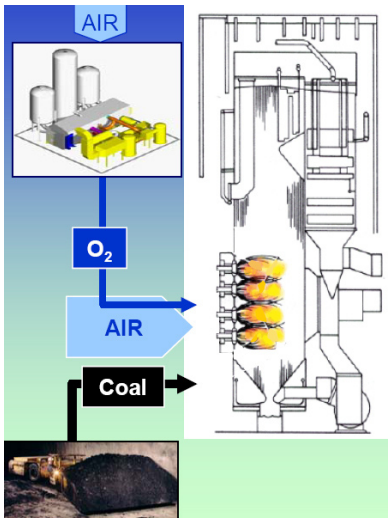
Objectives

Objectives for this project are separated into two phases.

Phase I objectives include:

- Evaluate the effect of coal rank that is currently used in existing boilers in an oxy-combustion design.
- Determine the equipment requirements for the boiler island for different coals and combustion systems.
- Investigate the potential for multi-pollutant (NO_x, SO_2, Hg, and particulate) reduction.
- Validate an existing 3-dimensional computational flow, heat transfer, and combustion model for oxy-combustion scale-up to a commercial size boiler.



Schematic for typical oxy-combustion process.

Phase II objectives are as follows:

- Conduct an engineering and economic assessment of the technology for commercial-scale retrofit application.
- Assess CO_2 control cost reductions via the integration of ASU flue gas purification, CO_2 compression train, CO_2 transportation, and sequestration.
- Evaluate the impact of oxy-combustion implementation on net power production and cost of electricity.
- Determine the boiler population with close proximity between stationary CO_2 sources and candidate geologic sink.

Benefits

This technology will play a part in moving the United States toward cleaner, more efficient power generation from coal and will help reduce costs of existing CO_2 capture systems. Through this project, Babcock & Wilcox expects to demonstrate a cost-effective approach for CO_2 capture, coupled with much lower nitrogen oxide emissions than normal coal combustion with air.

Accomplishments

- Process specifications, including CO_2 transportations & sequestration, flue gas purifications and storage were determined.
- A draft pilot plan has been submitted for testing of the oxyfuel system at a 6 MMBTU scale.

Planned Activities

- Test facility will be modified to a wall-fired configuration to determine the performance of the oxy-combustion process for this configuration.
- Test facility will be modified to a cyclone configuration to determine the performance of the oxy-combustion process for this configuration.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

IONIC LIQUIDS: BREAKTHROUGH ABSORPTION TECHNOLOGY FOR POST-COMBUSTION CO_2 CAPTURE

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Background

The University of Notre Dame and its partners are working to continue development of novel ionic liquid absorbents and an associated process for the removal of CO_2 from coal-fired power plant flue gas. Ionic liquids are salts that are liquid in their pure state near ambient conditions. In a previous NETL-funded project, Notre Dame demonstrated that ionic liquids can be engineered to have very high physical solubilities and can also be made to chemically complex CO_2. Due to their chemical diversity, ample opportunities should exist to tailor and optimize the properties of ionic liquids for CO_2 capture. Having shown their potential in the previous project, researchers will work in this project to take the next step in the development process.

Description

In Phase I, the University of Notre Dame will carry out atomistic-level computer simulations of a series of ionic liquids and functional groups along with flue gas species. This will give researchers insight into what chemical and structural features will lead to favorable properties. Simultaneously, researchers will investigate known CO_2 - phillic moieties, carry out synthesis of new ionic liquids, and make preliminary measurements of physical properties and phase behavior. We will also begin work on setting up the process model for the system. In Phase II, we will refine our development efforts for the "optimal" absorbent, exhaustively measure or estimate all relevant properties, and use this information to complete a detailed systems and economic analysis study. We will also design a lab-scale continuous absorption and regeneration system. During Phase III, we will construct and operate the lab-scale absorption and regeneration system, finalize process designs and develop a path forward for pilot-scale testing and commercialization.

Primary Project Goal

The overall goal of the project is to develop a new ionic liquid absorbent and accompanying process that enables 90% of the post-combustion CO_2 to be removed from a coal-fired power plant while attaining the 2012 capture cost target of less than a 20% increase in the cost of energy services according to the NETL Carbon Capture and Sequestration Systems Analysis Guidelines.

PARTNERS

University of Notre Dame
Trimeric Corporation
The Babcock and Wilcox Company
DTE Energy
Merck KGaA

PROJECT DURATION

03/01/07 to 06/30/10

COST

Total Project Value
$3,005,165

DOE/Non-DOE Share
$2,221,304 / $793,861

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Objectives

- Design and synthesize one or more ionic liquid absorbents having physical properties tailored for post-combustion CO_2 capture.
- Perform atomistic-level classical and quantum calculations to engineer ionic liquid structures that maximize CO_2 carrying capacity while minimizing regeneration costs.
- Measure or accurately estimate all physical properties of the ionic liquid that are essential for detailed engineering and design calculation.
- Complete a detailed systems and economic analysis.
- Demonstrate the CO_2 capture process with a continuous lab-scale unit.
- Develop a path forward for commercialization.

Benefits

If CO_2 capture is ever to become economically feasible, improved capture processes are needed. The use of ionic liquids as CO_2 absorbents holds promise for reducing costs by developing a process with higher CO_2 loading in the circulating liquid and lower heat requirements for regeneration. Both these effects would lower process costs.

Accomplishments

This is a new project. To date, researchers have initiated molecular modeling efforts and have already obtained quantitative agreement between simulated and experimental liquid densities for one ionic liquid. Researchers have also synthesized three new ionic liquids.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

CO_2 REMOVAL FROM FLUE GAS USING MICROPOROUS METAL ORGANIC FRAMEWORKS

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Background

UOP LLC, in collaboration with Vanderbilt University and the University of Edinburgh, is working to develop novel microporous metal organic frameworks (MOFs) and an asscociated process for the removal of CO_2 from coal-fired power plant flue gas. This innovative project will exploit the latest discoveries in an extraordinary class of materials (MOFs) having extremely high adorption capacities. MOFs have previously exhibited exceptional adsorption capacity for methane, hydrogen, and other gases. MOFs are hybrid organic/inorganic structures – essentially scaffolds made up of metal hubs linked together with struts of organic compounds, a structure designed to maximize surface area. MOF sorption properties can be readily tailored by modifying either the organic linker and/or the metal hub.

Description

The scope of this project is to develop a MOF-based CO_2 removal process and design a pilot study to evaluate the performance and economics of the process in a commercial power plant. During Phase I, UOP will use its combinatorial chemistry capabilities to systematically synthesize a wide range of state-of-the-art MOFs and related materials. UOP will screen the materials for hydrothermal stability and characterize materials of particular interest. Detailed isotherm data will be collected in the low pressure regime, in order to establish a consistent, relevant baseline for subsequent development and optimization. The results of the baseline studies will be used to guide the ongoing synthesis, screening and measurement of new MOFs. In Phase II, up to 10 candidates will be selected for optimization, based on Phase I results. The effects of water on CO_2 adsorption will be measured in parallel with the development and validation of material scale-up and forming procedures. During Phase III, one or two of the best materials will be selected for final optimization and scale-up to pilot-scale quantities. The effects of contaminants on the performance of scaled-up, formed materials will be optimized and detailed kinetic and equilibrium data will be collected. These data will be incorporated into a process design and process economic analysis, leading to the design of a pilot study.

Primary Project Goal

The objective of this project is to develop a low cost novel sorbent and the process around it to capture CO_2 from coal-based power plant flue gas in a cost-effective manner.

PARTNERS

UOP LLC
Vanderbilt University
University of Edinburgh

PROJECT DURATION

04/01/07 to 03/31/10

COST

Total Project Value
$2,802,200

DOE/Non-DOE Share
$2,230,672 / $571,528

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Objectives

- Phase I – Evaluate known MOF materials and enable down-selection to <10 candidate materials for further development based on CO_2 capacity and hydrothermal stability.
- Phase II – Further develop and test up to 10 MOF materials and demonstrate one or more MOF materials with improved performance and stability that are suitable for optimization and scaleup in Phase III.
- Phase III – Demonstrate one or more MOF materials that meet performance targets and have sufficient stability to carry into pilot testing.

Benefits

Current CO_2 capture technology imposes a significant cost burden on delivering electricity. The proposed technology has the potential to change the CO_2 capture economics, enabling practical CO_2 sequestration and accelerating the widespread use of CO_2 capture in the power-generation industry.

Accomplishments

This is a new project. During the first quarter, significant progress was made on the synthesis of MOF materials, as more than 10 materials were successfully prepared. The materials were characterized by conventional techniques such as x-ray diffraction, thermal gravimetric analysis, and high-resolution electron microscopy to ultimately enhance the understanding of relationships among material properties and CO_2 capture performance.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

BIOMIMETIC MEMBRANE FOR CO_2 CAPTURE FROM FLUE GAS

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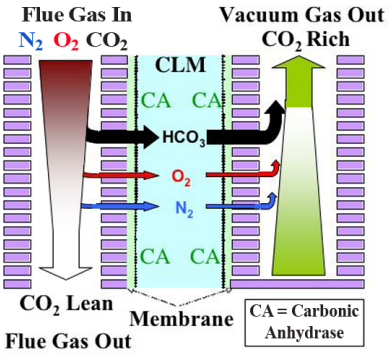
Background

Carbon Capture and Sequestration (CCS) is a three-step process including capture, pipeline transport and geologic storage of which the capture of carbon dioxide (CO_2) is the most costly and technically challenging. Current available methods impose significant energy burdens that severely impact their overall effectiveness as a significant deployment option. Of the available capture technologies for post combustion applications – absorption, adsorption, reaction and membranes chemically facilitated absorption promises to be the most cost-effective membrane solution for post combustion application.

The Carbozyme technology extracts CO_2 from low concentration, low pressure sources by means of chemical facilitation of a polymer membrane. The chemical facilitation is occurs through the use of a catalyzed Carbonic Anhydrase (CA), a carbonate-bicarbonate process that has exhibited, in the laboratory, lower parasitic loads than competing CO_2 capture technologies. CA is the fastest CO_2 catalyst known. The proposed process is applicable to both natural gas and coal-fired boilers.

Description

The performance of Carbozyme's enzyme-based CLM. technology depends upon more fully matching coal-based power plant operating conditions and economic constraints. This relies on appropriate use of the information on the chemical, physical and process-engineering characteristics of the enzyme based contained liquid membrane (EBCLM) design. This project addresses issues of particle management, permeator fluid condensation and increased operating temperature. These studies compliment previous work concerning the effects of acid gases on the contained liquid membrane (CLM).



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Carbozyme, Inc.

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Primary Project Goal

This project's overall objective is to develop a very cost efficient, low energy, CO_2 capture system (EBCLM) applicable to coal based power plant flue gas exhaust exhaust streams. The successful EBCLM permeator will have high CO_2 permeance and high selectivity while maintaining low energy requirements for regeneration. The overall energy consumption target is under 15 percent.

Objectives

- Characterize the effect of operating parameters on water condensation.
- Investigate CO_2 removal efficiency at low temperature using different enzymes.
- Investigate CO_2 removal efficiency at high temperature using CAM, a member of the γ-CA family of isozymes.
- Develop a preliminary commercialization plan.

Benefits

- The EBCLM provides absorption and stripping in a single modular, scaleable apparatus.
- The EBCLM green design uses fully biodegradable materials.
- The EBCLM has the potential to reduce the overall energy burden associated with carbon dioxide capture which will in effect lower the overall increase in the cost of electricity compared to competing technologies.

Accomplishments

- A temperature control system has been developed and demonstrated in the laboratory to abate evaporative condensation within the EBCLM. Abatement of the condensation is important because previous studies have demonstrated its potential to impede the flow within the hollow fiber membrane. This approach will limit temperature changes to a few tenths of a degree Celsius.
- Several different enzymes were examined to show a desired operating temperature range of 4 °C – 85 °C.

Planned Activities

A key next step is to scale the permeators and test them under controlled actual conditions to focus on the ability to manage the flue gas streams from different ranks of coal.

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

4/2008

FABRICATION AND SCALE-UP OF POLYBENZIMIDAZOLE - BASED MEMBRANE SYSTEM FOR PRE - COMBUSTION CAPTURE OF CARBON DIOXIDE

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Background

In order to effectively sequester carbon dioxide (CO_2) from a gasification plant, there must be an economically viable method for removing the CO_2 from other gases.

While CO_2 separation technologies currently exist, their effectiveness is limited. Amine-based separation technologies work only at low temperatures, while pressure-swing absorption and cryogenic distillation consume significantly large quantities of energy (up to 35 percent). In contrast, polymer-based membrane separations use much less energy and typically provide low-maintenance operations. Polymer membranes have been used successfully in a number of industrial applications, including the production of high-purity nitrogen (N_2), gas dehydration, removal of acid gases, and recovery of hydrogen (H_2) from process streams for recycle. However, successful use of a polymer membrane in synthesis gas separation requires a membrane that is thermally, chemically, and mechanically stable at high temperature and high pressure. Unfortunately, the commercially available polymeric materials currently employed are not sufficiently stable in such demanding environments.

In general, as operating temperatures increase, gas separation is significantly reduced and gas flow declines due to membrane compaction (creep). In addition, current membrane materials are often subject to chemical degradation by impurities in the process stream, a problem that is exacerbated by elevated temperature. Consequently, there is a compelling need for membrane materials that can operate under these more demanding environmental conditions for extended periods of time while providing a level of performance that is economically sustainable by the end user.

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PARTNERS

SRI International

Los Alamos National Laboratory

BP Alternative Energy

Southern Electric Company

Whitefox Technologies

Visage Energy

Enerfex

PERFORMANCE PERIOD

04/01/07 to 03/31/09

COST

Total Project Value
$5,083,854

DOE/Non-DOE Share
$4,047,695 / $1,036,159

Description

The system produced in this project will consist of a minimum of four membrane modules, a control system, and a skid. The system must be able to separate H_2 from CO_2 in a syngas feed stream that has undergone low-temperature water gas shift process. The size of the membrane modules will be sufficient to separate a syngas stream that has 0.25 MWth heating value. The system will be able to accommodate syngas feed streams ranging in temperature from 200 °C to 400 °C. The system will also be able to operate at feed pressures ranging up to 700 psi.

Primary Project Goal

The overall goal of this project is to develop a polybenzimidazole (PBI)-based capture system that is capable of operation under a broad range of conditions relevant to the power industry while meeting the U.S. Department of Energy's Carbon Sequestration Program goals of 90 percent CO_2 capture at less than a 10 percent increase in the cost of energy services.

Objectives

- One of the key milestones for the project will be to construct a capture system in a 3-year timeframe that can be field tested at an end user's facility.
- Acquire and test a polymer-based membrane—available commercially or reported in the literature—for separations involving hydrogen.

This achievement is validated via membrane productivity (separation factor and flux) comparisons (Figure 2). The improved performance of this technology in an application such as IGCC-integrated capture is further substantiated by the accessible operating temperature range (up to 400 °C), long-term hydrothermal stability, sulfur tolerance, and overall durability of the composite membrane materials in these challenging pre-combustion environments. Additionally, the modular, low-maintenance, and flexible design of the membrane technology, combined with the technology achievements anticipated over the course of the life of this project, make it an exceptional candidate for use for pre-combustion capture of CO_2.

Benefits

This project will produce step-change improvements in the cost and performance of gas separation technology.

Accomplishments

- The first generation (Gen1) of PBI-based hollow fibers have been produced and are being evaluated and optimized. The hollow-fiber platform offers a means to produce an economically viable, high area density membrane system amenable to incorporation into an IGCC plant for pre-combustion CO_2 capture.

- The Gen1, small-scale hollow-fiber-based membrane module has been designed and fabricated.

- The impact of membrane placement on process economics is under evaluation using ASPEN.

- Preliminary specifications and protocols for evaluations of the PBI-based fiber and membrane have been established.

- Market trends that may impact the successful commercialization of the PBI-based system for pre-combustion applications have been evaluated and reported.

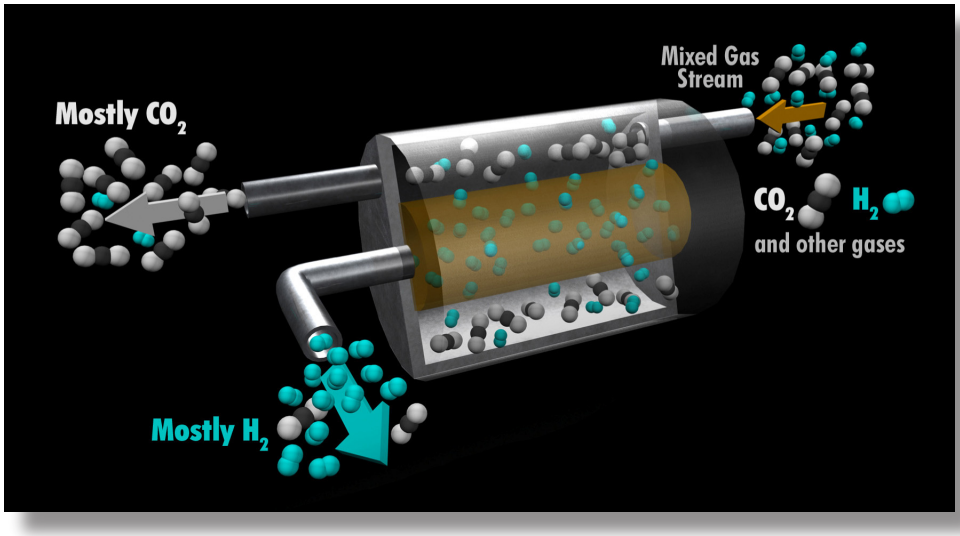

Figure 1. Simplified model of a single tube membrane module

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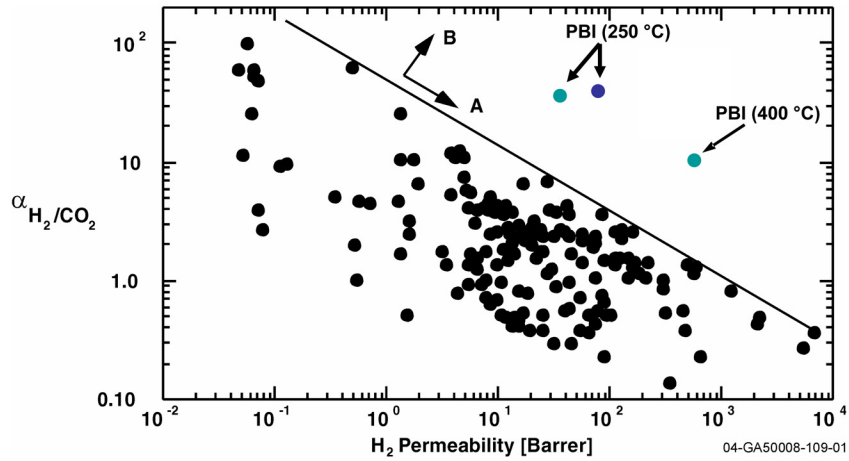
Selectivity vs. Permeability: H_2/CO_2



● = "wet" ● = "dry"

1 barrer = 10^{-10} cm^3-cm/s-cm^2-cmHg

We have demonstrated improved selectivity over the state-of-the-art while operating at industrially attractive conditions

From Polymer. (23) 35, L.M. Robeson, et al., 1994.

Figure 2. Compilation of literature data of membranes for separation of H_2 and CO_2. The line on the plot is called the "upper-bound" and is thought to be a limit of what is obtainable for a given separation with a polymeric material. The PBI in this investigation exceeds the "upper-bound" and falls into a commercially attractive regime.

Project472.indd

PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

DEVELOPMENT OF BIOMIMETIC MEMBRANE FOR NEAR ZERO PC POWER PLANT EMISSIONS

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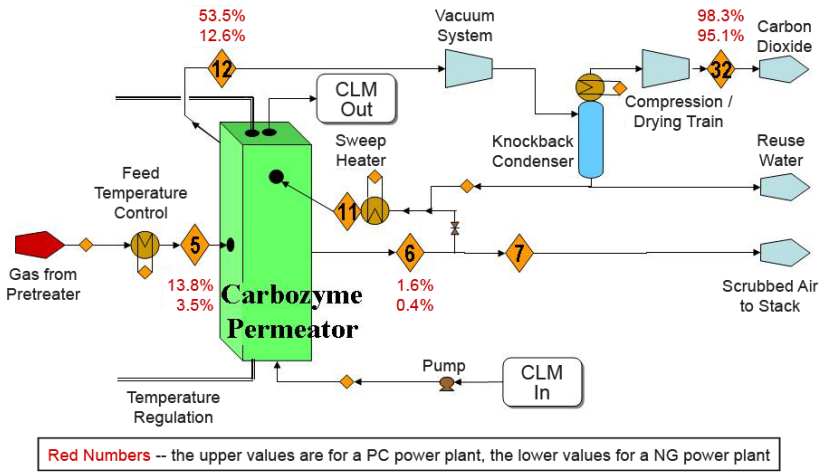
Background

CO_2 capture is the largest single cost element of the Carbon Capture and Sequestration (CCS) program, accounting for more than 65 percent of the total. Capture methods currently available impose significant energy cost burdens (parasitic loads) that severely impact their overall effectiveness. Development, system testing, and scale-up demonstrations of efficient, cost-effective methods for CO_2 capture are essential to enable wide-scale deployment at both existing and new power plants.

Description

The Carbozyme contained-liquid membrane (CLM) system leverages the most efficient CO_2 catalyst known, carbonic anhydrase (CA). CA rapidly converts CO_2, at very low energy, to bicarbonate at the flue gas interface and reverses the process at the CO_2 product interface. This process allows for efficient, simple, and scalable designs for the capture of CO_2 from low-concentration, low-pressure sources such as power plant flue stacks. In addition, the process is green technology because all of the materials are biodegradable or environmentally benign.



Process Engineering Schematic

Primary Project Goal

The goal of this project is to demonstrate the ability of an enzyme-based CLM permeator to efficiently extract CO_2 from a variety of flue gas streams, including coal and natural gas. The permeator performance will be considered successful if it achieves the DOE target values, at least 90 percent separation, and 95 percent

purity in the captured flue gas stream with a cost of energy of less than 20 percent by 2012. The project objective is to achieve a parasitic load of less than 15 percent. The proposed development work is expected to demonstrate progressive cost, performance, and feature improvements that will support acceptance of the CLM permeator system for both retrofit and greenfield power plants.

Objectives

The main objective of this project is to demonstrate and evaluate, at pre-pilot scale, the ability of the Carbozyme enzyme-based CLM permeator to capture CO_2 from a variety of combusted coal rank flue gas streams. Subsidiary objectives include:

- Development of a flue gas pretreatment system that meets the acceptance criteria for SO_x, NO_x, mercury, and particulates.
- Selection and commercial-scale development of a preferred enzyme variant (isozyme).
- Development and scale-up of the hollow fiber CLM permeator, culminating in a prepilot permeator skid that successfully removes CO_2 to the target goals.
- Development of a novel, enzyme-based electrodialytic prototype that demonstrates feasibility and improved performance, and that scales to a multi-cell stack to realize optimized system cost and efficiencies.
- Engineering and Economic Analysis of the CLM and electrodialytic technologies as they relate to retrofit and greenfield installations.
- Development of a commercialization study to provide a path to rapid introduction and application.

Benefits

The Carbozyme technology could provide power plants with a cost effective means to capture CO_2 from flue gas. The enzyme-based, CLM permeator has shown the promise of capturing CO_2 from simulated and actual flue gas streams at significantly reduced cost compared to an absorption technology, MEA.

Planned Activities

Successful scale-up of the Carbozyme technology will entail:

- Definition and identification of flue gas pretreatment systems with acceptable performance for the Carbozyme CLM CO_2 capture system.
- Development and validation of methods to produce CA enzyme on an industrial scale.
- Design and prototype of a fully scalable, modular, skid-based hollow fiber contained liquid membrane CO_2 capture system that can be arranged to fit most footprints, and has the ability to be built and staged off-site.
- Design and development of a fully scalable, modular, electrochemical CLM CO_2 capture system.
- Evaluation of multiple strategies for CO_2 capture, including assessments of efficiency, as well as capital and operating costs.
- Process engineering design activities in support of system scale-up.
- Comprehensive commercialization planning to help accelerate market entry.

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Novozymes NA
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Argonne National Laboratory
Visage Energy Corp.
SRI International
ElectroSep, Inc.
Kansas State University
KES Inc.
North Dakota Lignite Council
Cogentrix Energy, Inc
Otter Tail Energy
Great River Energy
Montana Dakota Utilities

PROJECT DURATION

03/28/2007 to 03/27/2010

COST

Total Project Value

$7,181,243

DOE/Non-DOE Share

$5,743,981 / $1,437,262

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R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Sequestration

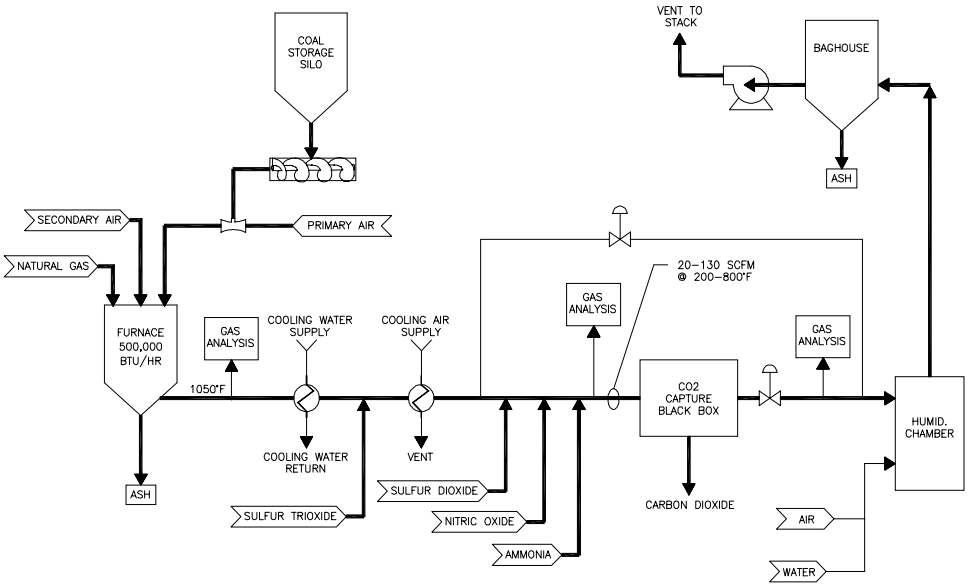
4/2006

Modular Carbon Dioxide Capture Facility

Capabilities

Carbon Sequestration is rapidly becoming accepted as a viable option to reduce the amount of carbon dioxide (CO_2) emitted from large point sources, while continuing to use our Nation's fossil fuels to produce affordable, clean energy. As a major step in a carbon sequestration scenario (storage being the other), the capture or separation of carbon dioxide represents a significant cost and energy penalty in the overall requestration process. To accelerate the development of low-cost capture and separation technologies, NETL is implementing the design and construction of a modular, flexible CO_2 capture test facility. The facility will be able to test new capture technologies on coal combustion flue gas and, additionally, on process gas from advanced fossil-fuel conversion systems, such as coal gasification. Ultimately, a database for a particular capture technology will provide experimental information from which further engineering scale-up decisions can be formulated.

In the flue gas mode, the Modular Carbon Dioxide Capture Facility (MCCF) will mimic coal-fired combustion processes that produce electricity. The combustor can be fired with natural gas, coal, or a combination of the two; coal-burning of approximately 40 pounds of pulverized coal per hour results in a flue gas (110-scfm) laden with various pollutants. The versatility of a "black-box" design will permit the incorporation of a particular capture/separation technology anywhere along the flue gas path. If regeneration of the capture medium is required as part of the capture/separation process, this step can be readily integrated into the system.



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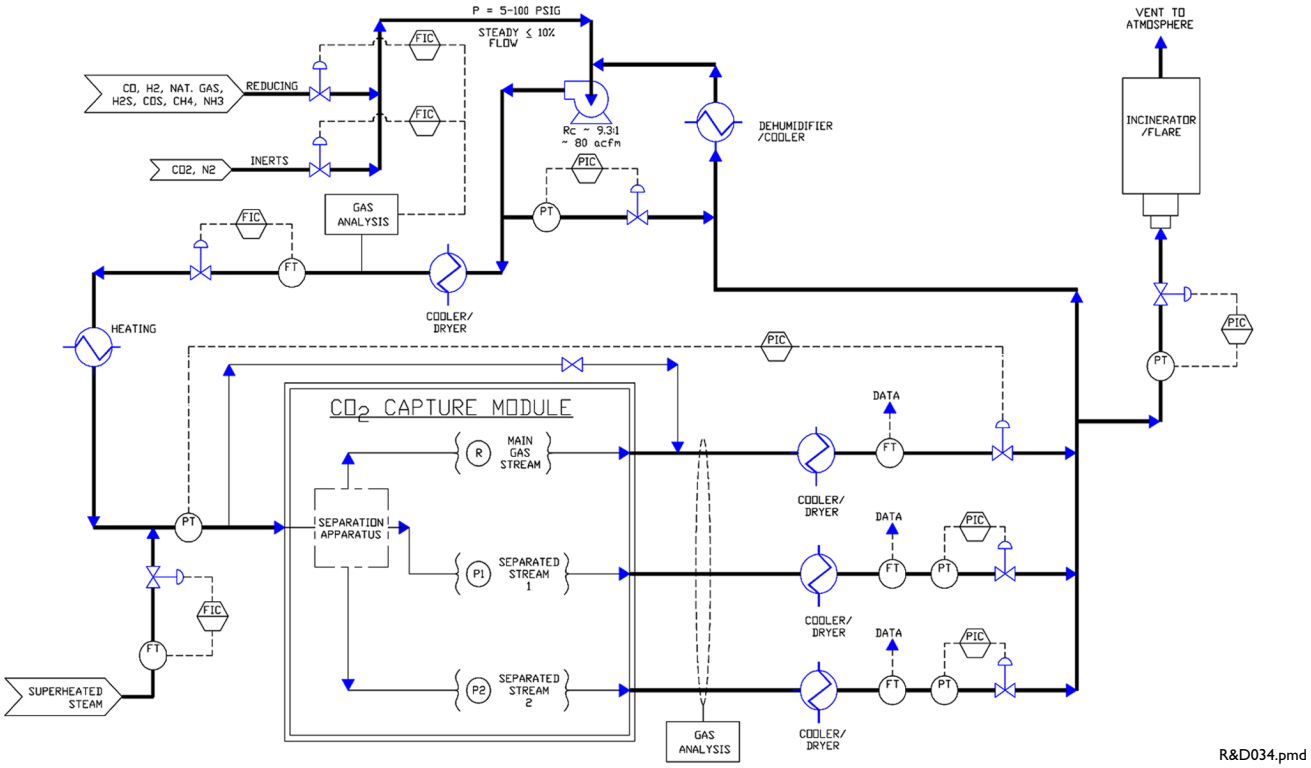
In a fuel gas mode, the MCCF will blend various high pressure gases (hydrogen, carbon monoxide, water, carbon dioxide, and minor components) to simulate the gas composition found in gasification processes, for example IGCC and Vision 21 plants. Again, a versatile design will permit installation of a capture technology, possibly including regeneration, along the fuel gas flow network.

By providing a means to evaluate the most promising capture/separation CO_2-abatement processes, the MCCF will help DOE meet its goal of developing point source cleanup systems that are more efficient, cleaner, and less costly than the current established techniques proposed for implementation in today's power generation plants.

Opportunities

- The MCCF has evolved as a multipurpose, versatile research facility.
- Performance of a particular carbon dioxide-abatement process can be optimized in the MCCF to help achieve the extremely high emissions-control goals of the DOE Carbon Sequestration program. Operational performance standards for CO_2 capture will thus be established.
- The MCCF provides the ability to test capture and separation concepts on process streams that simulate advanced energy conversion systems.
- Side-by-side comparison of advanced capture and separation concepts can be conducted.
- The MCCF can be used to investigate the impact of gaseous components (SO_2, NO_x, H_2S, particulates, and/or air toxics emissions) and other parameters on the particular technology.
- The MCCF offers industry and other sequestration stakeholders the opportunity to further develop CO_2 capture/separation technologies through cooperative ventures with the government (NETL). Collaborations with CO_2 capture technology developers will be sought.



R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

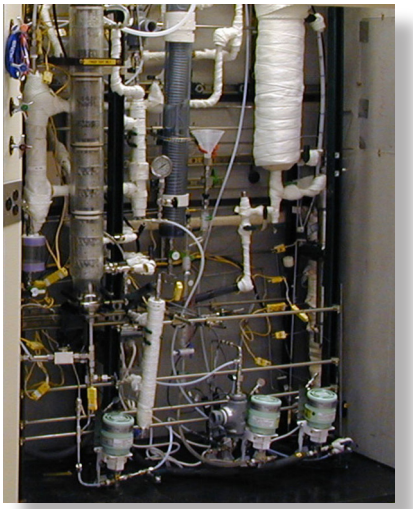
Carbon Sequestration

09/2007

Ammonia-based Process for Multicomponent Removal from Flue Gas

Background

Carbon sequestration is considered a viable method of reducing carbon dioxide (CO_2) emissions from large point sources. One point source, the pulverized coal-fired power generator, has been and will be in the near future the predominant power-generating technique. In response, NETL is developing an ammonia-based wet scrubbing process for capturing CO_2 in flue gas.



Continuous flow system for testing the ammonia-based process.

The project began as part of an international collaboration with China with an interest in the formation of ammonium bicarbonate fertilizer. However, as there is not a significant market for this type of fertilizer in the United States, NETL recognized the need to develop an ammonia-based scrubbing technology as a regenerable process. In an effort to control multiple acidic gases (e.g., CO_2, SO_2, NO_X, HCl) plus fine particulates from flue gas produced by coal-burning power plants, NETL proposed the use of an ammonia-based process that is regenerative in terms of CO_2 capture for carbon sequestration. While the ammonia solution is used to produce ammonium sulfate and ammonium nitrate by-products for fertilizer production, the ammonium bicarbonate solution is heated to release high-purity CO_2, which will be sequestered. The other product of the regeneration step, ammonium carbonate solution, is recycled in the process and reused to absorb more CO_2. The regenerative CO_2 capture chemistry is described by reversible chemistry between the ammonium carbonate and ammonium bicarbonate in an aqueous solution:

$$(NH_4)_2CO_3 + CO_2 + H_2O \leftrightarrow 2\ NH_4HCO_3$$

Although commercial ammonia-based processes exist for the removal of SO_2 and NO_X from flue gas, NETL developed this additional scrubbing capability for CO_2 capture.

Primary Project Goal

The primary goal is to select a regenerable CO_2 carrier with high CO_2 carrying capacity. The process must be energy efficient, and the new robust carrier must not be degraded by O_2 or SO_2, NO_X, and other acidic gases that exist in the fossil fuel combustion flue gases.

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Objectives:

Major objectives are to:

- Search for a carrier that has overall lower parasitic power loss than other carriers (commercially available monoethanolamine).
- Develop a process to clean criteria pollutants from flue gas and generate salable by-products, such as fertilizers, that could offset the costs of sequestration.
- Develop a single-solvent process for multicomponent control of flue gas emissions.
- Ensure the process is technically and economically feasible through a systems analysis.
- Collaborate via a CRADA with an industrial partner, Powerspan Corp., utilizing their experience with ammonia scrubbing to further develop the process.
- In partnership with the University of Pittsburgh, develop a process simulation model to aid in process scale-up to commercial size.

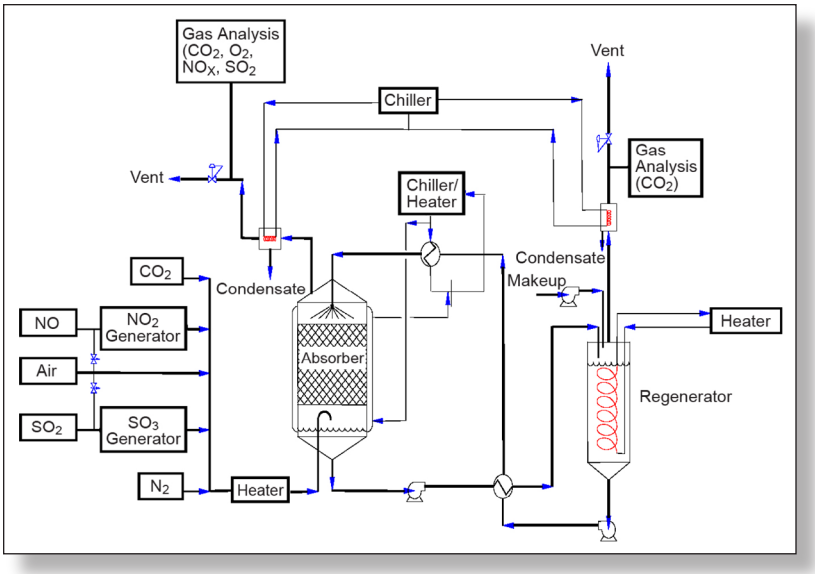
Accomplishments

A continuous flow closed-loop reactor was designed and constructed, and parametric tests were performed. The effects of process operating parameters on CO_2 removal efficiencies were analyzed and reported. These quantification/optimization tests established major impacts of these parameters on CO_2 carrying capacity, ammonia losses, and ammonium species. Major ammonium species in the reactor were identified, and it was determined that excessively high temperatures during regeneration should be avoided to reduce ammonia gas loss.

Benefits

Because of the widespread use of coal to produce power, an alternative scrubbing technique is needed to further capture CO_2 in flue gas. Ammonia-based scrubbing can produce technical and economic benefits compared to current scrubbing technologies. From the experimental information to date, lower parasitic energy consumption, the production of a salable fertilizer, and the capability of one solvent to remove many components are just some of the reasons that the ammonia-based process will be a significant technology in the carbon sequestration area.

Powerspan's demonstration plant in Shadyside, OH, already cleans coal combustion flue gas to remove mercury vapor, SO_2, and NO_x .



Continuous process flow diagram.

R&D043.indd

R & D facts

U.S. Department of Energy
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Carbon Sequestration

04/2008

Solid Sorbents for CO_2 Capture from Precombustion Gas Streams

Background

According to the President's Global Climate Change Initiative as described in NETL's carbon sequestration technology roadmap and program plan, CO_2 capture from coal gasification systems is critical for the Department of Energy's CO_2 sequestration program. Current commercial CO_2 capture technology is expensive and energy intensive. In addition, most of the techniques require gas cooling for CO_2 capture, which contributes to the loss of thermal efficiency. It is important to develop low-cost processes that utilize materials with high CO_2 adsorption capacity, high selectivity for CO_2, high diffusivity, high rates of adsorption, and high rates of regenerability.

Primary Project Goal

The primary goal of this research project is to develop regenerable sorbents that can capture CO_2 from high-pressure gas streams from such sources as coal gasification systems and are superior to existing commercial technologies.

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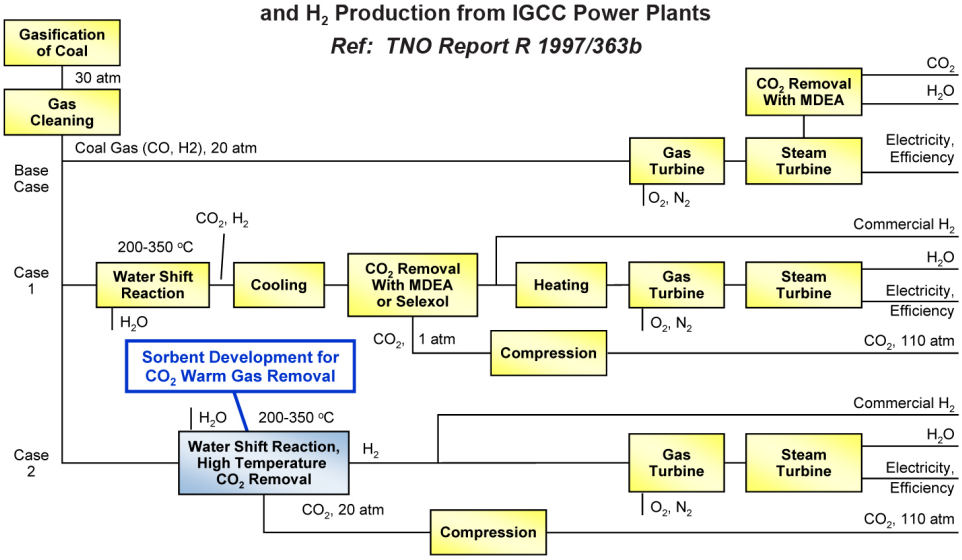
Comparison of Different Options for CO_2 Removal and H_2 Production from IGCC Power Plants

Ref: TNO Report R 1997/363b



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PROJECT PARTNERS

Süd-Chemie Inc. (Louisville, KY)

Carnegie Melon University (Pittsburgh, PA)

COST

Total Estimated Cost
$25,000 per year

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Objectives

The major objective of this work is to develop solid regenerable sorbents that have high rates, selectivity, high regenerablity, and high sorption capacity for precombustion CO_2 capture. Specific objectives include:

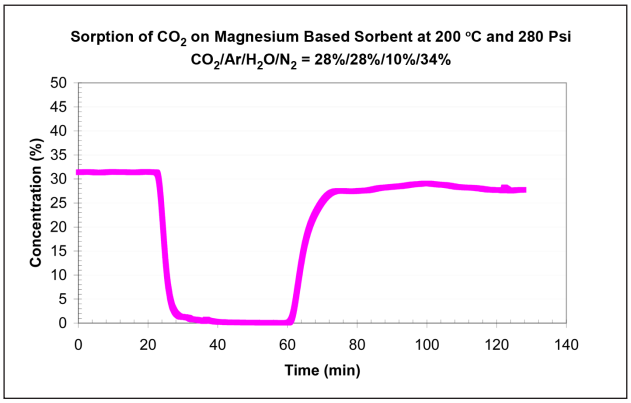
- Develop regenerable sorbents that operate at higher temperatures suitable for CO_2 capture from precombustion gas streams, such as those from Integrated Gasification Combined Cycle (IGCC) systems.
- Conduct a complete system analysis incorporating sorbent-enhanced water-gas shift reaction.
- Test and evaluate the feasibility of utilizing the sorbent for sorbent-enhanced water-gas shift reaction.

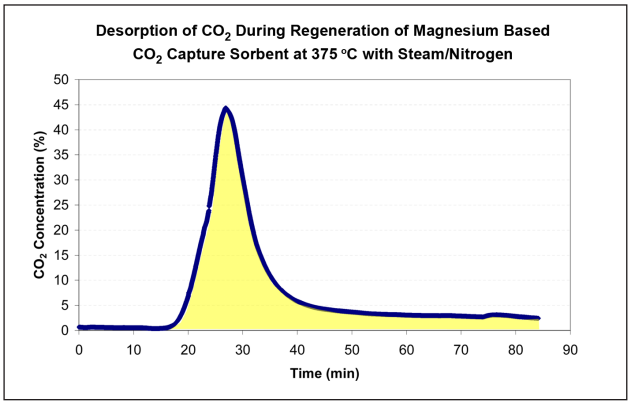
Accomplishments

- Regenerable sorbents that can capture CO_2 at water-gas shift reactor temperatures were successfully developed.
- High pressure CO_2 capture and high pressure regeneration were demonstrated.
- A U.S. patent for the NETL-developed, high-temperature CO_2 capture sorbent has been awarded.
- The evaluation of zeolites for higher-temperature applications was completed and the good CO_2 capture capacity at 120 °C observed. Process optimization studies and model development with zeolites were completed in collaboration with Carnegie Mellon University.

Benefits

Development of a cost-effective CO_2 capture technology suitable for coal gasification systems is necessary to achieve the President's Global Climate Change Initiative without increasing the cost of electricity from coal.





R&D046.indd

R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Sequestration

4/2006

Mechanistic Study of CO_2 Adsorption on Solid Amine Sorbent

Background

The capture of CO_2 from gas mixture can be achieved by using solvents, cryogenic techniques, membranes, and solid sorbents. Amine-based, wet scrubbing systems have been used as capture techniques for CO_2 removal from flue gas streams. The possible reaction sequences in an aqueous system using primary and secondary alkanolamines reacting with dissolved CO_2 are shown in Figure 1.

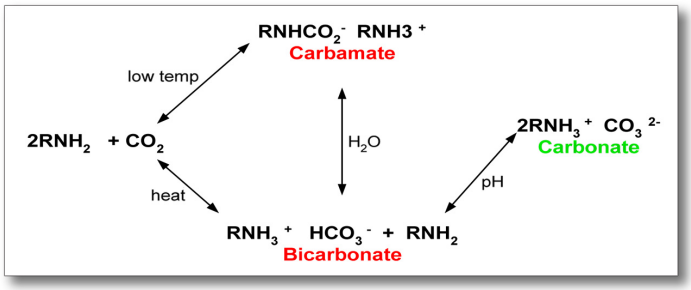


Figure 1. Possible reaction sequence for the capture of carbon dioxide by liquid amine- based systems.

According to Figure 1, the majority of the CO_2 captured will result in the formation of bicarbonate in these liquid amine capture systems. In aqueous media, there is a requirement of 2 moles of amine/ mole of CO_2 for the formation of stable bicarbonate compounds resulting in the capture of CO_2. For the case of solid amine sorbents, the detail reaction sequence is unclear thus far.

One strategy to develop a high CO_2 adsorption capacity solid sorbent is to graft amine functional group(s) containing species on the high surface area supports. A high surface area support will allow us to graft a higher number of active amine sites per gram of support. The nature of the grafted amine functional groups (primary or secondary amine) will determine the amount of CO_2 adsorbed and the energy required for regenerating the sorbent. The interaction between the CO_2 and NH/NH_2 groups is expected to be stronger than van der Waals forces but weaker than a covalent/ionic bond such that the CO_2 bound to the amino groups can be released with temperature swing. In order to fabricate a high CO_2 capture capacity solids amine sorbent, we must understand the fundamental interactions between CO_2 and amine on solid surface.

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Primary Project Goal

The goal of the research is to determine what factors affect the efficiency of the solid CO_2 sorbents.

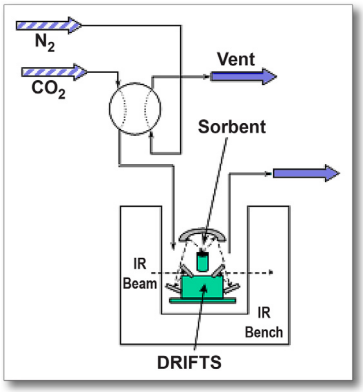

Figure 2. An assembled apparatus included a diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) cell for sorption/desorption measurements.

Objectives

- Use infrared (IR) spectroscopy to investigate the mechanism of CO_2 adsorption/desorption on amine sorbents;
- Estimate the effect of moisture content on the adsorption kinetics and sorption capacities of amine sorbents.

Accomplishments

IR study of the interactions between CO_2 and amines:

The experimental work for carbon dioxide interaction with 3-propylamine functionalized gel was initiated by using infrared spectroscopy. Infrared spectra of an Aldrich 36,425-8 sample and 3-propylamine functionalized silica gel were grafted on mesoporous SBA-15 particles which were collected repeatedly using two complete regeneration cycles. The cycles were collected at different partial pressures of carbon dioxide in nitrogen and demonstrated a fairly reproducible correlation between the free CO_2 gas concentration and the intensity of the signal corresponding to various adsorbed species. The amount of the weakly bound bidentate bicarbonate was directly related to the partial pressure of CO_2. Some carbonate complexes were not easily removed, even at 90 °C. Carbamate formation becomes a dominant mechanism of adsorption on 3-propylamine at higher CO_2 pressures.

Procedure:

- Prepare Aldrich 36,425-8 sample, 20 mg for FTIR analysis
- Outgas in N_2 at 90 °C for 4 hrs.
- Ambient T, N_2
- Ambient T, Switch to CO_2
- Ambient T, Switch to N_2 to remove CO_2
- Repeat cycle with regenerated sample

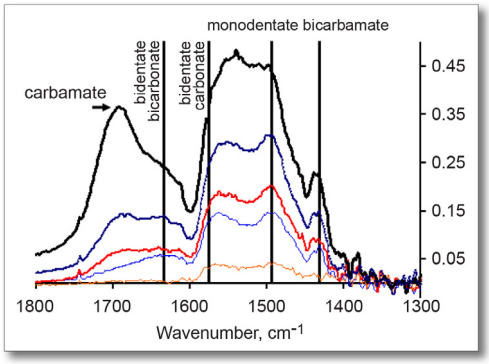

Figure 3. The amount of the weakly bound bicarbonates is directly related to the partial pressure of CO_2. Some carbonate complexes are not as easily removed, even at 90 °C. Carbamate formation becomes a dominant mechanism of adsorption on 3-propylamine at high CO_2 pressures.

Benefits

The separation process in aqueous amines is effective for carbon dioxide adsorption but it presents a corrosion and degradation problem involving extensive energy use for regeneration of the amine solution. The solid sorbent, in addition to elimination of these problems, may offer an advantage of high surface area density available for adsorption. This may also enhance the fundamental knowledge of CO_2-amine interactions on solid sorbents.

R&D053.pmd

R & D facts

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National Energy Technology Laboratory

Carbon Sequestration

09/2007

Molecular Design of CO_2 Ligands Ionic Liquids and Poly (ionic liquids)

Justification and Background

The potential for various ionic liquids (ILs) and poly(ionic liquids) (PILs) to capture CO_2 is being investigated. Papers published by Radosz and co-workers indicate that PILs can have very larger CO_2 uptake compared with ILs. One of their most surprising results was that four of the IL monomers they tested had essentially zero uptake capacity for CO_2, whereas when polymerized, the corresponding PILs showed very large uptake at a temperature of 22 °C and a pressure of about 0.8 bar. Molecular modeling combined with COSMOtherm is being used to gain insights into these surprising findings

Approach

Turbomole ab initio calculations have been used to predict the σ profiles for the following PIL/IL pairs: PVBIH/VBIH, PVBIT/VBIT, PBIMT/BIMT, PVBTMA/VBTMA, PMATMA/MATMA, PVBBI/VBBI and on the [bmim][BF4] and other ionic liquids. In cooperation with an industrial researcher, COSMOtherm calculations using the σ profiles have been used to estimate the Henry's law constants and solubilities for CO_2 in the ILs and PILs at the experimental condition of 22 °C and 0.8 bar. Results from these calculations are summarized in Table 1. Good agreement for some of the PILs and ILs tested have been found but there are discrepancies for several systems. Therefore an experimental program has been initiated to confirm the computational results.

Table 1. Experimental and calculated CO_2 solubilities for various poly(ionic liquid)s.

Poly(ionic liquid)s	Experiments	Calculations
PVBTMA+BF_4	10.2	2.2
PMATMA+BF_4	8.0	1.2
PVBIH+PF_6	2.7	3.3
PVBBI+Tf_2N	2.2	3.1
VBBI+Tf_2N	N/A	3.0
PVBIT+BF_4	2.2	2.7
PBIMT+BF_4	1.8	1.9
BIMT+BF_4	1.3	1.8
bmim+BF_4	1.3	1.7
VBIH+PF_6	0.0	3.1
VBIT+BF_4	0.0	2.5
VBTMA+BF_4	0.0	0.7
MATMA+BF_4	0.0	1.0

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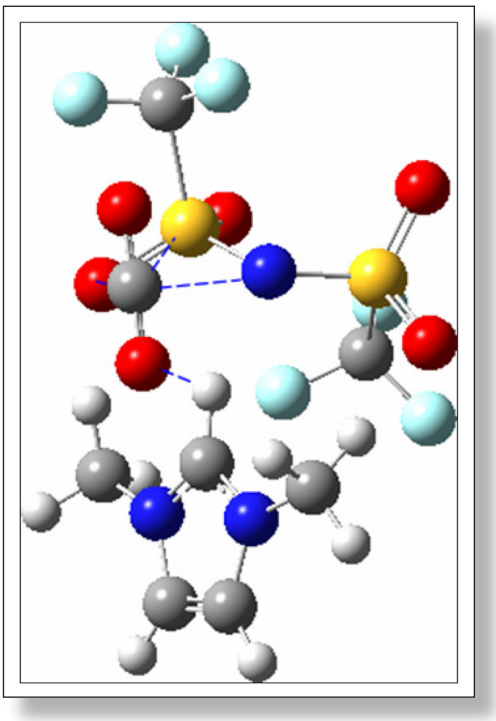
Project Goal

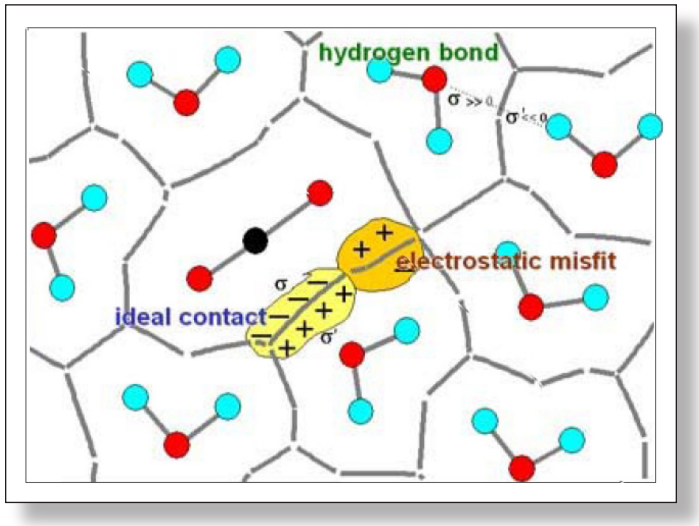
Develop ionic liquids or poly (ionic liquids) to be used as sorbents or membranes which will allow a decrease in the cost of carbon dioxide capture from coal-based power generation to such extent that 90 percent of the carbon dioxide produced may be captured, transported and sequestered at less than a 10 percent increase in the cost of the energy services.

Expected Benefits

Development of an ionic liquid/poly (ionic liquid) model capable of accurately predicting material properties will guide the application of these ionic liquid based materials to membrane and sorbent development for CO_2 capture.



CO_2 binding with the anion (Tf2N)



COSMO-RS is a theory that describes the interactions in a fluid as local contact interactions of molecular surfaces. The interaction energies are quantified by the values of the two screening charge densities σ and σ' which form a molecular contact.

R&D120.indd

R & D facts

U.S. Department of Energy
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Carbon Sequestration

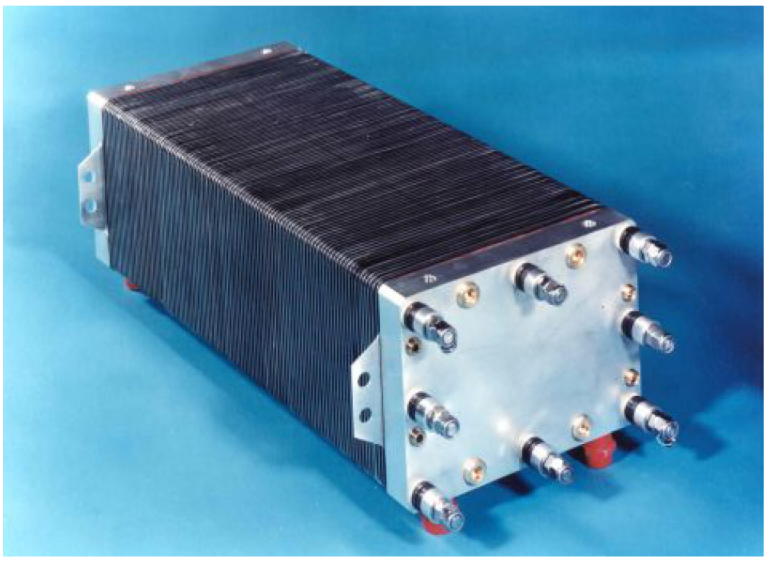
08/2007

Electrochemical Separation of CO_2

Background

The project described in this work plan will investigate novel technology options to enable reductions in CO_2 emissions for wide range of applications. The goal of the proposed work is to investigate concepts using electrochemical devices to separate and compress carbon-dioxide. However, there are several research issues that need to be addressed prior to achieving this goal.

Electrochemical separation and compression of CO_2 is a relatively new area. Prior literature has suggested electrochemical separation using carbonate ion pumps. Electrochemical separation/compression technologies are also a new research area. In the last decade, several other electrochemical separation/compression concepts have been described for gases like hydrogen and oxygen. It has been suggested the electrochemical hydrogen compression as a novel hydrogen compression category. In fact, there are a substantial number of reports in the open literature of using electrochemical devices to simultaneously separate and compress gases, particularly hydrogen which has been compressed to 5,000 psi using an electrochemical device.



Possible future device for electrochemical CO_2 separation

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The electrolytes used for carbonate fuel cells are somewhat limited, and in many cases, these electrolytes are corrosive. The most popular electrolyte requires an operating temperature in the range of 600 °C. In order to achieve the goals of this project, lower temperature electrolyte materials are required. Some of these electrolytes may have to be developed. This effort will collaborate with Carnegie Mellon University and the University of Pittsburgh on the development of electrolyte materials for separating carbon-dioxide for oxy-fired combustion. The limited ion-flux across existing electrolyte materials is a critical issue for this concept. The feasibility of an electrochemical separation device must address these limitations. For this reason, a new concept will be pursued to enhance the ion transfer through the electrolyte.

Objectives

- **Assess Concept To Improve Ion Conductivity For Electrochemical Device**

  The purpose is to investigate a novel concept to improve the ion conductivity through an existing YSZ device.

- **Assess Options for Electrochemical Device Development Laboratory**

  The purpose is to assess the possible alternatives for building and testing electrochemical devices that can simultaneously separate and compress CO_2. The laboratory should also have the capability to test electrochemical devices that can recover energy from "waste" heat streams in fossil-fuel applications.

Benefits

- Develop an effective electrochemical cell for CO_2 removal that can be inexpensively produced.

- Integrate electrochemical separation into advanced fossil fuel power plant concepts.

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R & D facts

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Carbon Sequestration

09/2007

Solid Sorbents for CO_2 Capture from Powerplant Exhaust Streams

Background

Current commercial CO_2 capture technology (e.g., gas absorption by solutions of carbonates and alkanolamines) is expensive and energy intensive. It is important to develop low-cost processes that utilize materials with high CO_2 adsorption capacity, high selectivity for CO_2, high diffusivity, high rates of adsorption, and high rates of regenerability.

Primary Project Goal

The primary goal of this research project is to develop regenerable sorbents that can capture CO_2 from coal combustion systems and are superior to existing commercial technologies.

Objectives

The major objective of this work is to develop solid regenerable sorbents that have high rates, high selectivity, high regenerablity, and high adsorption capacity for postcombustion CO_2 capture in suitable conditions. Specific objectives include:

- Develop sorbents for various reactor designs.
- Evaluate the feasibility of sorbent preparation in commercial-scale units and bench-scale reactor tests.
- Develop regeneration schemes to obtain a concentrated CO_2 stream.
- Optimize the sorbent formulation to improve sorbent performance.
- Conduct long-term tests to determine the chemical and physical stability of the sorbents.
- Study the effect of trace contaminants on the sorbent performance.
- Test the sorbent in a pilot-scale reactor unit.

NETL CO_2 sorbent extrudates prepared at a commercial facility (Süd-Chemie Inc.)

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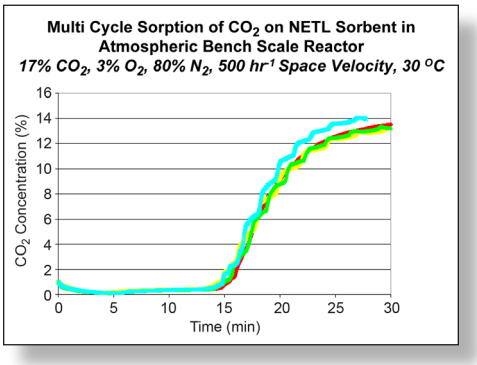
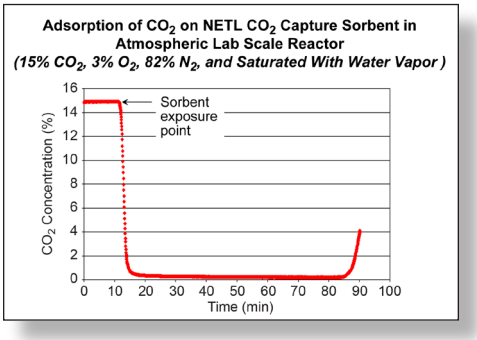
Accomplishments

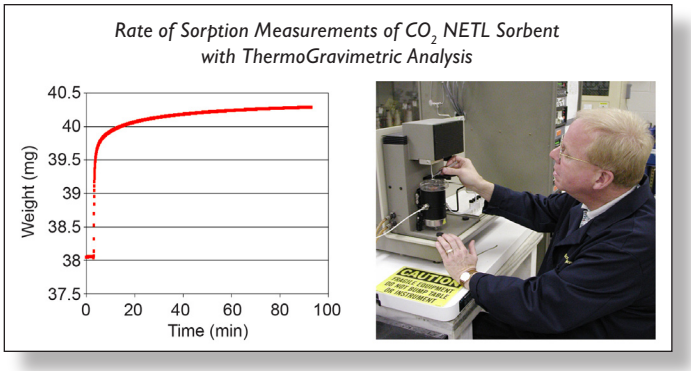
During the project, solid sorbents suitable for CO_2 capture from coal combustion gas streams were developed. Different types of sorbents are being evaluated for use. In one approach, liquid impregnated solid sorbents that capture CO_2 in the presence of water vapor at temperatures from 30–60 °C have been developed. In another approach, amines compounds capable of capturing CO_2 have been attached to various substrates, and the capture capacity for CO_2 has been measured in laboratory experiments. The sorbents showed better CO_2 capture capacities and lower regeneration temperatures than the conventional amine-based liquid solvent scrubbing process. A large-scale preparation of one of the sorbents at a commercial company was conducted successfully, and the sorbent showed promising results during bench-scale flow reactor tests with simulated coal combustion gas streams. The sorbent has CO_2 removal efficiency of 99% with good removal capacity. Continuing studies are quantifying how the sorbents perform in simulated operating cycles for both absorption and regeneration, with the goal of optimizing the sorbent performance for specific reactor configurations. A separate NETL study is evaluating the options for designing a reactor to use these sorbents in an actual reactor configuration.

Benefits

The majority of coal combustion power plants do not capture CO_2 and the current adaptable commercial processes are very expensive. Development of a cost-effective CO_2 technology is necessary to achieve the President's Global Climate Change Initiative with minimal increase in the cost of electricity from coal.







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R & D facts

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National Energy Technology Laboratory

Carbon Sequestration

09/2007

Reactor Design for CO_2 Capture Using Sorbents

Background

Carbon Sequestration is rapidly becoming accepted as a viable option to reduce the amount of carbon dioxide (CO_2) emitted from large point sources (for example, power generation plants), while continuing to use our Nation's fossil fuels to produce affordable, clean energy. The capture or separation of carbon dioxide from flue gas represents a significant cost and energy penalty in the overall sequestration process. Solid sorbents for CO_2 capture are one option to reduce the penalty associated with capturing flue gas CO_2. In addition to the sorbent development, specific reactor configurations must be developed to manage the flue gas flow, and the sorbent handling and regeneration. The project will facilitate commercial readiness of advanced, cost-effective sorbent-based capture technologies. Technical challenges include identification of candidate reactor designs with sorbents for investigation. Once identified, engineering design criteria must be provided to determine the applicability of the technology in a power generation scheme.

Objective

The project seeks to obtain the optimal design and engineering information for sorbent-based technology. Engineering support and reactor design oversight will be provided for the development of CO_2 removal processes utilizing solid sorbents currently under development by NETL researchers. The sorbent technology will ultimately reach the programmatic goal to be able to remove 90 percent CO_2 while keeping the increase in cost of energy service below 10 percent for post-combustion techniques.

Accomplishments

Based on an external study related to CO_2 sorbent development, the initial performance target for CO_2 capture with sorbents from flue gas is a reduction of 30-50 percent of the energy required for a wet scrubbing MEA process. Key engineering information (heat of reaction, specific heats, loading capacity, moisture effects, etc.) will be experimentally obtained for candidate in-house sorbents being developed. This information combined with isotherm studies will be used to update the reactor analysis of this external study.

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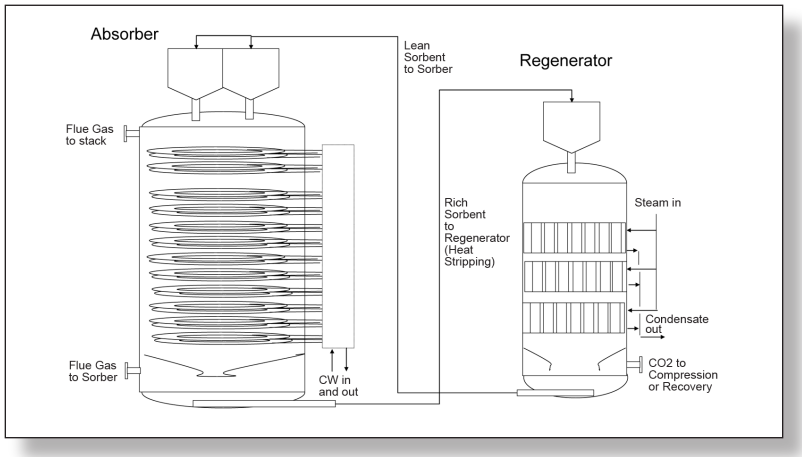
Detailed modeling of both the absorber and regenerator will be performed by university researchers through university consortium partnerships and in-house NETL modelers. The efforts are focusing on management of heat and mass transfer for various reactors configurations, including reactors proposed in an external study. Insertion of chemical kinetics into the modeling effort will also be included. In addition to examining moving and fluid bed concepts, another design under consideration is the use of a transport reactor system.

Key Results to Date Include:

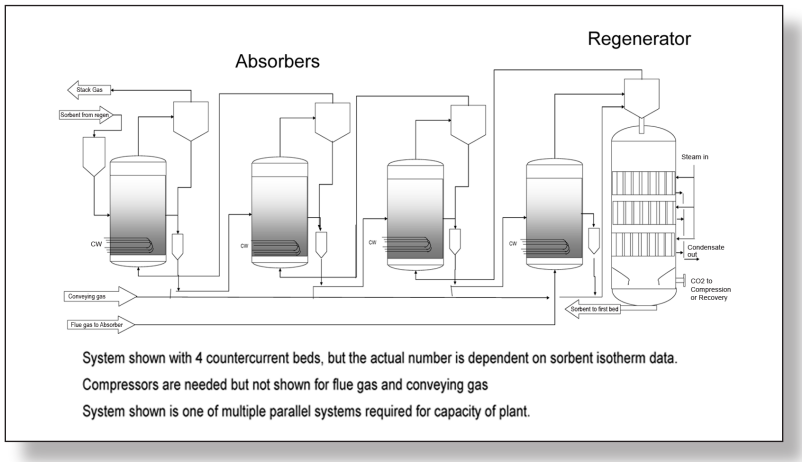
- Measured sorbent parameters play a significant role in the type of reactor that is suited to the application, showing tradeoffs in sorbent properties for fixed-bed, moving-bed, or fluid bed concepts.
- Heat management is critical in both the absorption and regeneration process, and will require significant heat transfer surface in contact with the sorbent.
- Down-selection has produced four conceptual reactor designs.

Benefits

Because of the widespread use of coal to produce power, a novel scrubbing technique is needed to further capture CO_2 in flue gas. Sorbent-based scrubbing can produce certain technical and economic advantages as compared to more traditional wet scrubbing processes. However, the use of the sorbent in a particular reactor design is a key and will ultimately determine whether the realization of a sorbent-based technology can indeed be used for CO_2 capture from flue gas.



Moving Bed Reactors



Fluid Bed / Moving Bed Reactors

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R & D facts

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Carbon Sequestration

08/2007

Novel CO_2 - Philic Absorbents

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Summary

The ability to separate a high pressure mixture of CO_2 and H_2 such that a high pressure stream of CO_2 for sequestration *and* a high pressure stream of H_2 for energy are produced remains an elusive goal. This research has identified a class of compounds that melt in the presence of high pressure CO_2, forming a liquid phase composed of roughly 50wt% CO_2 and 50wt% of the compound. Unlike conventional solvents that require substantial depressurization during regeneration to release a low pressure CO_2 stream, these novel compounds completely release the CO_2 at many hundreds of psia as the compound solidifies. This work will reveal whether one of more of these compounds can selectively remove CO_2 from a mixture of CO and H_2 at high pressure and release the CO_2 after a modest depressurization.

Problem

One version of an IGCC plant gasifies coal and then employs the water-gas shift reaction to produce a high pressure process stream that is rich in CO_2 and H_2. It would be advantageous to process this mixture such that it simultaneously yields a high pressure CO_2 stream for geologic sequestration and a high pressure H_2 stream for the generation of electricity. Commercial separation technologies, such as membranes, PSA and gas absorption columns, have the ability to produce high pressure CO_2 or high pressure H_2, but not both. The goal of this work is to determine if the ability of novel CO_2 - philic compounds (that liquefy and absorb significant amounts of high pressure CO_2, and then release the CO_2 via a very small pressure drop that causes the compound to solidify) can be used to establish a separation process that yields a high pressure hydrogen stream and a high pressure CO_2 stream.

Methodology

It is anticipated that prior work in CO_2 - philic solids, coupled with molecular modeling contributions (which recently helped us to design new CO_2 - philic compounds), will lead to the development of a truly unique CO_2 - solvent. Prior research identified two classes of compounds, sugar acetates and tert-butylated aromatics, that are extremely "CO_2 - philic". Examples of sugar acetates include glucose pentaacetate and maltose octaacetate, and examples of tert-butylated

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aromatics include tri-tert-butylbenzene and tri-tert-butylphenol. Tri-tert-butylphenol (TTBP) is a commercially available compound (~$3/lb) that is a solid at room temperature with a melting point (in the absence of CO_2) of 135 °C. In the presence of CO_2 at 50 °C and a pressure of about 1500 psia, the TTBB melts and a liquid phase containing as much as 50wt% TTBP forms. This liquid phase can be slightly depressurized to a slightly lower pressure, roughly 1450 psia, in order to produce a solid TTBP powder that contains no CO_2 and a high pressure CO_2 phase that contains trace amounts of TTBP. Similar experiments conducted with pure H_2 demonstrate that these compounds do not experience a similar melting point depression; these compounds are not H_2 - philic.

Our intention is to exploit this property for the separation of a CO_2 - H_2 mixture. If the TTBP is capable of selectively absorbing CO_2 from the mixture, the process would yield a H_2 - rich gas stream and a TTBP - CO_2 high pressure liquid. The TTBP - CO_2 liquid could be slightly depressurized to release 100% of the CO_2 as the solid TTBP forms. However, this process would have to deal with the handling of solid particulate TTBP.

The objectives would be to determine (using TTBP as an example) the phase behavior of TTBP - CO_2 over a wide range of T, the phase behavior of TTBP - H_2 over the same range of temperature, the separation of H_2 and CO_2 over a wide range of temperature, pressure, gas composition, and gas-TTBP ratio. During this experimentation, various configurations of IGCC cycles would be examined to determine the optimal placement of this separation system, which (based on our preliminary results) appear to be high pressure and relatively low temperature (below 300 °C).

Expected Outcomes

- The phase behavior of CO_2, H_2, CO_2+H_2 mixed with the CO_2 - phile (e.g., TTBP) can be determined from non-sampling visual phase behavior experiments or from sampling VLE experiments.
- Proof-of-concept gas separations can be conducted using either closed systems (in which pressure changes could be used to monitor gas absorption or release) or open systems that would introduce and withdraw a gas stream from the vessel that contains the solid or molten TTBP (in which the composition of the gas in the vessel and/or the effluent gas would be determined using GC).

R & D facts

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Carbon Sequestration

09/2007

Surface Immobilization Nanotechnology for CO_2 Capture

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Summary

Carbon dioxide is considered to be one of the major greenhouse gases directly influencing global climate change. It is estimated that 36% of the United States' anthropogenic CO_2 is produced from coal/fired power plants. Consequently, the capture and sequestration of CO_2 from flue gas streams is an essential step for carbon management in the environment.

The capture and separation of CO_2 can be achieved by using solvents, cryogenic techniques, membranes, and solid sorbents. Among them, aqueous amine solutions have been widely used. Although an amine solution is effective for CO_2 absorption, it presents a corrosion problem to equipment and it degrades through oxidation. However, solid sorbents offer a number of advantages, including low energy requirement for sorbent regeneration, and elimination of corrosion problems. The development of an economic CO_2 separation process requires a highly efficient CO_2 sorbent. The sorbent must possess high CO_2 - capture capacity, long-term use and the ability to be regenerated with a small difference in adsorption and desorption temperatures. One potential approach for preparing such a sorbent is to graft CO_2 adsorption sites on a high surface area support. Obviously, the more adsorption sites grafted on the surface, the higher the capacity for CO_2 capture. Therefore, a new technique for immobilizing high amounts of amine compounds, which are accessible by CO_2, on the same substrate surface is needed to develop low-cost and highly-efficient solid sorbents for CO_2 capture.

This project will take full advantage of the electrostatic layer-by-layer self-assembly (LBL) technique, which is a very useful and novel nanotechnology for fabrication of multilayer coatings. LBL nanotechnology has the following advantages:

- The process provides a novel approach to develop ultrathin coatings on any shape of substrate at room temperature.
- The coating can be very stable.
- Different materials can be assembled in a pre-designed order.
- The process is relatively straightforward and can be automated and scaled-up for mass production.
- The process is environment-friendly.
- The process allows super-molecular structures to be built with molecular control.
- The process permits control of coating thickness, uniformity and roughness on the nanometer scale.

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Approach

Several approaches have been investigated for CO_2 capture, and among them, amine grafted solid sorbents have shown great promise. However, the amount of amines that can be immobilized is still relatively small, and further enhancement of CO_2 capture capacity is beneficial. The long-term goal of this research is to reduce the release of greenhouse gases to the atmosphere from flue gas streams by developing novel technologies for CO_2 capture. The rationale is that the proposed nanotechnology provides a novel approach for grafting substantially larger amounts, for instance 100 times more, of amine compounds and also possibly other polymers than currently studied solid sorbents. This study will lead to the development of highly-efficient and multi-functional novel solid sorbents.

Expected Benefits:

The electrostatic layer-by-layer self-assembly (LBL) is the most promising method for preparation of multilayer nanocoatings of controlled thickness and molecular architecture. Novel sorbents are expected to be developed using this nanotechnology, and the developed sorbents will have the following features:

- Low-cost: the LBL process is simple, and the amines (e.g., PEI, PAA) used are cheap.
- Highly-efficient: extremely high amounts of amine compounds, for example 100 times the currently studied sorbent systems, will be immobilized on the sorbent as a porous multilayer coating.

Expected Outcomes:

A multidisciplinary collaboration has been established to conduct the proposed project. The team includes an Assistant Professor at WVU as principal investigator (PI), a Professor at Pitt, and a Scientist at NETL. This team is particularly well-prepared to undertake the proposed research. This is because the collaboration will take advantage of the complementary expertise of the PI in nanotechnology and bioengineering, of the CO-PI in reactor/process design as well as modeling, and of the NETL scientist in physics and chemistry. The success of the project will result in further collaborations, not only on the development of novel sorbents but also on the development of novel membrane systems, among the NETL and the regional universities. This will enhance the in-house research at NETL.

R & D facts

U.S. Department of Energy
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Carbon Sequestration

09/2007

Development of Metal Organic Framework Materials for CO_2 Separation

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Summary

There are at least three different applications where separation of CO_2 from other gases is of interest. These are: 1. Separation of CO_2 from fuel gas (output from gasification, water gas shift reactors, etc.); 2. Separation of CO_2 from sour natural gas wells (natural gas containing large fractions of CO_2); and 3. Separation of CO_2 from flue gas. These separations must each be accomplished very cost effectively if sequestration is to be a viable technology, yet each has distinct requirements. For example, the CO_2 partial pressure and concentration is relatively low for the last application and therefore chemical-strength binding may be required to capture CO_2 from flue gas. To examine the potential of metal organic framework (MOF) materials for the ability to act as highly selective membranes for separation of CO_2 is proposed. This is a multi-scale problem that will require collaborations with researchers at NETL doing experimental work on synthesis and testing of MOFs and with university teams doing various levels of modeling, from detailed quantum mechanics to continuum-level approaches.

Problem:

Metal organic frameworks are crystalline materials that can be tailored to specific applications through varying the metals, ligands, and linkers making up the MOF. They can be synthesized inexpensively, relatively easily, in high purity, and in a highly crystalline form. The number of potential MOFs is virtually limitless, as changes in the ligands, secondary building blocks, or the linkers will produce novel MOF with distinct properties. Experimental characterization of a large number of different MOFs is a very expensive and time-consuming procedure. Therefore, significant progress could be made if computational methods could be applied to help screen candidate materials. In the best case scenario, computer simulations would be used to design new MOFs based on required performance of the material. This project is a first step toward computational design of functional MOFs. The main goals of the research are: (1) develop a detailed characterization of the interaction between CO_2 and a number of existing MOFs; (2) compute adsorption isotherms and transport diffusivities of pure and mixed gases in various MOF from atomic-scale simulations; (3) develop a macroscopic model for transport of gas mixtures through a model MOF membrane; and (4) identify candidate structures that increase the selective permeability of CO_2 through MOF membranes.

Methodology:

The most important aspect for numeric prediction of MOF behavior is the interaction potential model used in the simulations. Validation will occur with the potential models (Lennard-Jones parameters, point charges, etc.) to be used in the calculations and refinement of the potentials where needed by using highly-accurate ab initio molecular orbital and density functional theory methods. Potentials are needed

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for the framework atoms interacting with a number of adsorbates, including CO_2, N_2, O_2, H_2, CO, H_2O, and CH_4. Particular attention will be paid to the electrostatic interactions between the MOF and the adsorbate molecules. The electrostatic interactions are expected to be especially important for accurate modeling of CO_2 adsorption and transport. Once accurate potentials are in hand, Monte Carlo and molecular dynamics simulation techniques will be used to compute the adsorption of gas mixtures in and diffusion through MOF crystals. The initial work will focus on existing MOFs, such as MOF5 and Cu-BTC. Adsorption isotherms will be compared with experimental data for pure gases measured at NETL. Equilibrium molecular dynamics will be used to compute the self- and corrected diffusion coefficients, similar to methods used in previous work. Transport diffusivities will be computed from corrected diffusivities using adsorption isotherm information, computed from MC simulations. As an example the transport diffusivities calculated are shown in Figure 1 for H_2 in a novel zinc-based MOF (Zn[bdc][ted]) synthesized by Jing Li's group at Rutgers. It is critical to use molecular simulations to test assumptions that will be used to develop the continuum-scale model. The continuum-scale Maxwell model will be used for computing selective permeance through hypothetical MOF membranes. This continuum-level model will link the atomic-level simulations to experimental data, allowing us to assess how well various MOFs will perform under ideal conditions. It is critical to compare with experimental data as we generate simulation data on adsorption isotherms and diffusivities. Our recent work indicates that MOFs must be very carefully synthesized and activated (removal of solvent molecules) in order to achieve good agreement between simulations and experiments for adsorption isotherms. Moreover, electrostatic interactions between the framework and the adsorbate molecules can, in some cases, be very important. Therefore, development of potentials will be carried out in conjunction with experimental work measuring adsorption isotherms.

Once potential models have been developed, atomic and continuum-level computational techniques will be used to screen many existing materials for use as membranes that selectively transport CO_2. The ultimate goal of this work is to use computational methods to suggest new structures or chemical modifications to existing structures that will enhance the capability of MOFs to selectively transport CO_2. Design of new materials will require ab initio calculations and may involve use of software such as COSMO-RS, which can be used to relate the properties calculated from ab initio to thermodynamic properties such as Henry's law constants. Work will be confined to the physisorption regime. Chemisorption, as may be required for flue gas separation, will not be considered in this initial proposal.

Expected Outcomes

- An atomic-level picture of the potential for MOFs to separate CO_2 from various gas mixtures.
- A detailed characterization of the interactions between CO_2 and MOF and how that interaction might be controlled.
- Increased information from experiments due to modeling/experimental collaboration.
- The first detailed predictions of the performance of MOFs as gas separation materials.
- Quantitative comparisons of multiple MOF materials to guide experimental studies of MOF thin films.
- Quantitative study of the impact of lattice flexibility on gas solubility and diffusion in MOFs.
- Examination of possible applications of MOFs as components in polymer/MOF.

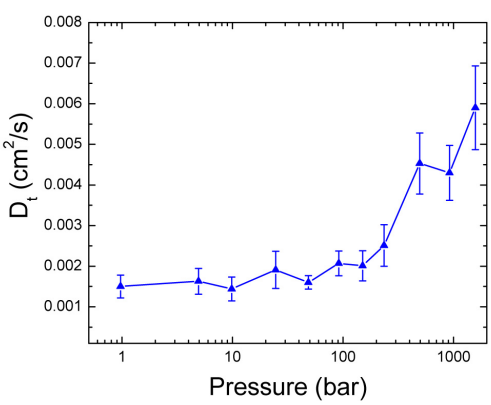

Figure 1: Transport diffusivities of H_2 in MOF Zn[bdc][ted] as a function of bulk gas pressure.

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R & D facts

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Office of Fossil Energy
National Energy Technology Laboratory

Carbon Sequestration

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Oxy-Fuel Combustion

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Objective

The overall objective of this project is to assist in improving and validating modeling tools for designing and improving oxy-combustion systems for new plants and retrofitting existing power plants. The result of this project will be that NETL has the capability to analyze retrofit and new oxy-combustion plants, to predict performance, and to recommend measures to improve performance.

Background

Oxy-fuel combustion is being developed for both turbine power cycles, and for pulverized coal plants. The products of oxy-fuel combustion are just carbon dioxide, and water. The water is easily separated, producing a stream of CO_2 ready for sequestration.

Pulverized coal oxy-fuel combustion burns fossil fuels in a mixture of recirculated flue gas and oxygen, rather than in air. The remainder of the flue gas, that is not recirculated, is rich in carbon dioxide and water vapor, and is a good candidate for treatment to condense the water vapor and capture the CO_2. An optimized oxy-combustion power plant will have ultra-low emissions.

Oxy-fuel power cycles can use coal syngas containing both CO and H_2 for combustion in a turbine cycle. Temperatures are controlled by recycled water (or CO_2) in a complete power system.

In both pulverized coal and power cycle applications, the current state of art is such that a greenfield oxy-combustion plant could be built or an existing plant retrofitted using existing technologies. However, such plants would not be optimized due to a lack of data or proven computer models of oxy-fuel combustors, boiler systems or carbon dioxide recovery systems. Multiple oxy-combustion facilities at various scales are being constructed or are in operation around the world. NETL is currently commissioning a lab scale burner suitable to study basic features of oxy-fuel combustion. These facilities are generating data that could be paired with NETL's expertise in the application of computer modeling. An objective of this project will be to develop cooperative relationships with the entities operating these facilities and to obtain data on oxy-combustion systems to supplement the NETL computational efforts.

Prior research on PC oxy-fuel has shown that, in order to maintain the oxygen/recirculated flue gas flame so that the oxy-combustion system has heat transfer characteristics similar to that of an air-fired system, an oxygen level of about 30-35% is required in the gas entering the boiler. Plants that are retrofit to oxy-combustion

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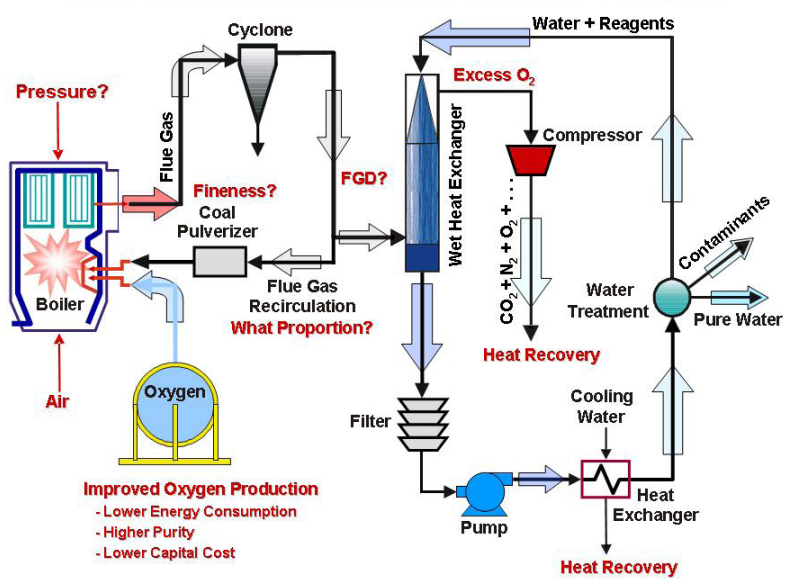
would likely operate within the range of oxygen levels that will maintain combustion conditions near those of air-fired systems. New oxy-combustion plants or repowered plants will not necessarily be constrained to be like air-fired systems, and more efficient designs will undoubtedly be conceived. The critical parameter of oxygen content may, for example, be adjusted to increase radiative heat transfer at the expense of convective heat transfer in zones further from the flame. In both retrofit and new systems, the changes inherent in oxy-combustion affect flame behavior; heat transfer; mass transfer; combustion gas chemistry and behavior; char burnout; slag development, chemistry, and deposition; and many other characteristics of fossil fuel combustion systems.

In a prior in-house project, heat recovery was identified as significant to improving efficiency of PC oxy-combustion systems. During processing of the combustion gas for carbon capture, sensible and latent heat in the exhaust gas and heat of compression can be partially recovered and returned to the plant via feed water. However, the changes in heat balance can lead to out-of-design conditions and the potential for failure. The low-pressure turbine was specifically identified as a vulnerable point. Also in prior projects, it has been shown that oxy-fuel power cycles would benefit from fundamental data on oxy-fuel gas-phase flame properties, such as flame speeds and radiant heat transfer.

As a result of the challenges identified by earlier NETL efforts in the oxy-fuel/ CO_2 - capture environment, other objectives of this project are to: 1) develop a better understanding of the oxy-combustion flame, and of heat and mass transfer in oxy-combustion systems; 2) develop an understanding of the character and distribution of ash and slag in PC oxy-combustion systems; 3) develop solutions for the potential low-pressure steam turbine imbalance in PC retrofit applications; and 4) support development of improved systems and CFD models and modeling tools.

An approach combining modeling, lab tests, and field work will be utilized. Development of relationships with other research entities will provide opportunities to conduct field evaluations of oxy-combustion test systems, which will positively impact all of the tasks of this project.



Gas path processes and areas for analysis.

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R & D facts

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Carbon Sequestration

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Chemical Looping for Combustion and Hydrogen Production

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Objective

The objective of this project is to determine the benefits of chemical looping technology used with coal to reduce CO_2 emissions.

Background

Chemical looping is a new method to convert coal or gasified coal to energy. In chemical looping, there is no direct contact between air and fuel. The chemical looping process utilizes oxygen from metal oxide oxygen carrier for fuel combustion, or for making hydrogen by "reducing" water. In combustion applications, the products of chemical looping are CO_2 and H_2O. Thus, once the steam is condensed, a relatively pure stream of CO_2 is produced ready for sequestration. The production of a sequestration ready CO_2 stream does not require any additional separation units and there is no energy penalty or reduction in power plant efficiency.

The majority of the work performed to date on chemical looping has been performed using methane as the fuel. There are only limited studies with oxygen carriers used to react with coal or gasified coal.

Project Description:

The project combines laboratory studies of "oxygen carriers" with models of chemical looping processes to determine how chemical looping can be used with coal. In prior work, a comprehensive literature search was performed to identify those chemical looping processes that involve coal gasification. Various oxygen carriers, including NiO on bentonite and CuO on bentonite have been prepared and evaluated as oxygen carriers at 700, 800 and 900 °C using thermal gravimetric analysis (TGA). Stable reactivity was observed over 10 cycles of oxidation with air and reduction with synthesis gas. Rate information was computed for reactions over both oxygen carriers. It was shown that particle size, temperature, and pressure affected the rate. Performance of these oxygen carriers were evaluated in a high pressure flow reactor at 150 psi with synthesis gas at 700, 800 and 900 °C. Stable reactivity was observed over 3 high pressure cycles, and complete combustion of hydrogen and complete utilization of the metal oxide were observed. Novel nano-composite oxygen carriers were also developed in collaboration with the University of Pittsburgh to improve the rates. The rate information is now being used to develop system level models of the chemical looping process, as well as

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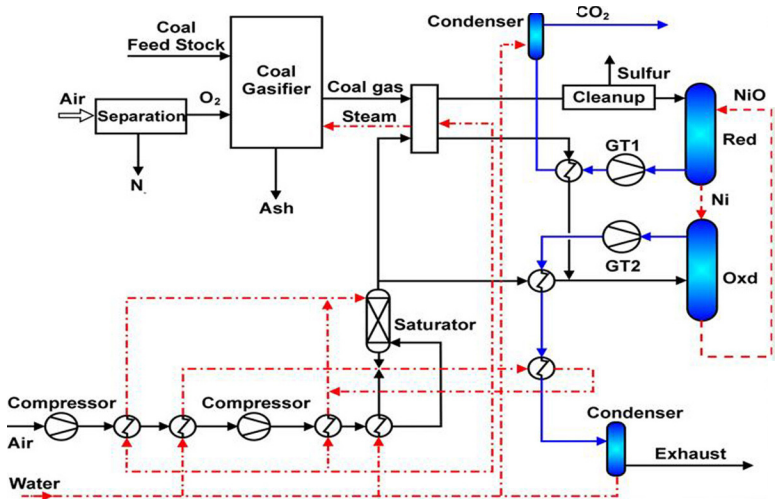
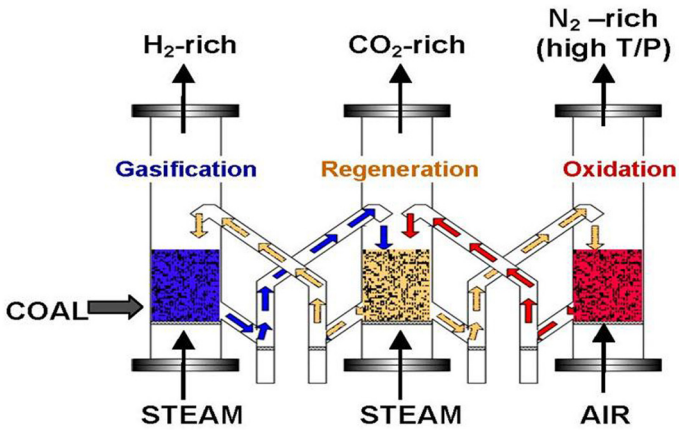
detailed Computational Fluid Dynamics (CFD) simulations of the chemical looping process itself.

Benefits:

Chemical looping can use coal to produce both hydrogen from coal, or a stream of combustion products that primarily consist of CO_2 and steam. A relatively pure stream of CO_2 that is sequestration ready can be produced by simply condensing the steam. This avoids the energy penalty traditional fossil fuel fired systems must pay to produce a pure stream of CO_2. Additionally, Chemical Looping for Combustion (CLC) minimizes production of NO_X that is produced in almost all other combustion processes.



Integrated gasification combined cycle with chemical looping combustion.



Fuel flexible gasification-combustion technology for production of H_2 and sequestration-ready CO_2 by GE Global Research.

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