U.S.-China Clean Energy Research Center

ACTC Research Areas:

Advanced Power Generation ................................................................. 2
Clean Coal Conversion Technology ...................................................... 5
Pre-Combustion CO$_2$ Capture ............................................................. 7
Post-Combustion CO$_2$ Capture ........................................................... 10
Oxy-Combustion CO$_2$ Capture .......................................................... 14
CO$_2$ Sequestration ............................................................................... 17
CO$_2$ Utilization .................................................................................. 21
Simulation and Assessment ................................................................. 24
Advanced Power Generation

Research Topic: 1

Research Objective
The researchers are pursuing activities that will lead to a breakthrough in advanced coal generation and applications of key technologies. There are three categories within this research topic:

Upgrade pulverizing system for subcritical power plants
- Evaluate potential improvements of coal pulverizers in coal-fired power plants (CFPPs) in China and the United States
- Identify target units from CFPPs with a coal classifier
- Improve fundamental understanding of dense fluid flows so as to lower NO\textsubscript{x} emissions

Advanced ultra-supercritical (A-USC) power generation
- Conduct research on combustion and heat transfer characteristics of large-capacity and high-parameter boilers
- Study the combustion and heat transfer characteristics of super 700°C A-USC boilers
- Establish a prediction model for ash deposition, and provide quantitative data for fine particle removal and ash deposition prevention

Improve efficiency, availability, and emissions reduction of existing CFPPs
- Obtain detailed data related to increasing efficiency and carbon reduction for different boiler types, loads, and coal types for in-service power plants
- Evaluate the retrofitting technologies and obtain the technological roadmap for increasing efficiency and pollutant emission reduction
- Obtain the retrofitting and operation experience of key technologies

Technical Approach
The technical approach for this project contains three categories:

Upgrade pulverizing system for subcritical power plants
- Survey the modification of coal pulverizers in CFPPs in China and the United States
- Evaluate potential improvements, including different configurations of coal mills and the pulverizing system
- Identify target units from CFPPs with a coal classifier
- Use a classifier lab rig in Beijing and modeling in Beijing and in WVU to improve fundamental understanding of dense fluid flows

A-USC boiler development
- Conduct research on a thermodynamic system of 700°C A-USC units combusting Xinjiang coal
- Design a system for 700°C A-USC boilers combusting Xinjiang coal

U.S. Research Team Lead
- Matt Zedler, LP Amina

U.S. Partners
- LP Amina

China Research Team Lead
- Yao Qiang, Tsinghua University

China Partners
- Tsinghua University
- Shanghai Jiao Tong University
- Harbin Institute of Technologies
- Huaneng Clean Energy Research Institute
- China Power Investment Corporation
- China Power Engineering Consulting Group Corporation
- Shenhua Group

Improved efficiency, availability, and emissions reduction of existing CFPPs
- Obtain detailed data related to increasing efficiency and carbon reduction for different boiler types, loads, and coal types for in-service power plants
- Evaluate the retrofitting technologies and obtain the technological roadmap for increasing efficiency and pollutant emission reduction
- Obtain the retrofitting and operation experience of key technologies

Technical Approach
The technical approach for this project contains three categories:

Upgrade pulverizing system for subcritical power plants
- Survey the modification of coal pulverizers in CFPPs in China and the United States
- Evaluate potential improvements, including different configurations of coal mills and the pulverizing system
- Identify target units from CFPPs with a coal classifier
- Use a classifier lab rig in Beijing and modeling in Beijing and in WVU to improve fundamental understanding of dense fluid flows

A-USC boiler development
- Conduct research on a thermodynamic system of 700°C A-USC units combusting Xinjiang coal
- Design a system for 700°C A-USC boilers combusting Xinjiang coal

• Conduct research on heat transfer and hydrodynamics of 700°C A-USC boilers
• Conduct research on fouling and slagging characteristics of 700°C A-USC boilers

**Improve efficiency, availability, and emissions reduction of existing CFPPs**

• Survey operation of existing CFPPs that have adopted efficiency improvement technology both in China and the United States
• Identify one or two specific units (e.g., 300–600 megawatt electrical [MWe]) with similar characteristics in both countries
• Analyze the operational characteristics and cycling behaviors of these plants and conduct a performance diagnosis
• Evaluate the potential for efficiency improvements and emission reduction
• Develop a final toolbox for both China and the United States to use in improving CFPPs
• Use CFD to study the effects of coal type and coal pulverization fineness on boiler emissions

**Recent Progress**

In 2012, research focused on investigating the combustion of Xinjiang Houxun coal in A-USC boilers. Fundamental experiments were conducted on coal with severe combustion characteristics. The development of improved A-USC boiler technologies was adopted as a national program by China. Also in 2012, LP Amina was able to investigate the current fuel processing system distribution in the United States. Further details on research progress include the following:

• Gathered statistics about type of unit, number, and capacity of CFPPs in China through a survey. The data showed that by the end of 2009, subcritical power plants account for 78% of the coal-fired fleet, while supercritical and ultra-supercritical units make up the remaining 22%. It was determined that the target plant for detailed investigation will be a subcritical unit with a capacity range from 300–600 MWe
• Finalized the benchmark investigation survey for the target CFPPs, with the following parameters necessary for a complete investigation: design parameters such as steam parameters, furnace and burner design, pulverizing system characteristics, flue-gas temperatures, and soot blowing system details; operational parameters such as heat rate, excess air, and load factor; and information about installing existing energy conservation and emissions reduction technologies such as soot blowing
• Carried out research on pulverized coal combustion in counterflow flames quite successfully. Accomplished the design, processing, assembly, and preliminary test of the first-of-a-kind experimental system

![Figures 1 and 2. Particle behavior during flame penetration is visible.](image)

• Studied the ignition in the Hencken burner and investigated different ignition mechanisms, ignition characteristics with a thermogravimetric analyzer/wire mesh reactor, and burnout properties of mixed coal. The research of A-USC power generation was combined with an investigation of the characteristics of Xinjiang coal. Research on combustion and hydrodynamic coupling characteristics of an A-USC boiler was performed. Theoretical modeling and numerical simulation of the aerial dynamic field, temperature field, and combustion efficiency of an A-USC boiler was completed. Construction of an experimental platform designed to investigate the combustion and hydrodynamic coupling characteristics of a 0.3 megawatt A-USC boiler is in process. The team also conducted an investigation on the transformation of minerals in combustion and the characteristics of soot heat resistance. The influence of fouling and slagging on the heat resistance of the heating surface was studied. To identify a methodology for predicting and controlling fouling and slagging, quantum chemistry was introduced

---

ACTC Fact Sheets  
Page 3  
November 2014
• Investigated the transformation of minerals in combustion and the characteristics of soot heat resistance. The influence of fouling and slagging on the heat resistance of the heating surface was studied. To identify a methodology for predicting and controlling fouling and slagging, quantum chemistry was introduced.

• Investigated the influence of the pulverizing system on NO\textsubscript{x} emission; researchers noted that the characteristics of the fuel, the primary air, and the combination of the air and fuel are the dominant influences. Factors such as the oxygen concentration in the burner zone and temperature in the burner zone also affect the emission of NO\textsubscript{x}.

*Expected Outcomes*

The research team’s efforts in A-USC power generation will produce a thermal calculation method of large-capacity and high-parameter boilers, a general large-capacity boiler thermal calculation program module, a calculation method of furnace combustion and heat transfer for super 700°C A-USC boilers, heat transfer coupling characteristics between the furnace and the pipe of USC boilers, and a prediction model of ash fouling and slagging in A-USC boilers.
Research Objective

Collaborative research teams from the United States and China are performing research and development (R&D) of new coal co-generation systems with CO$_2$ capture, including new coal-to-chemical co-generation; new CO$_2$ capture processes; and co-generation systems with combined pyrolysis, gasification, and combustion. Specifically, the team will accomplish the following:

- Develop and deploy a new poly-generation technology to reduce waste heat, water utilization, and greenhouse gas emissions while improving thermal efficiency in utilization of coal to produce power and chemical by-products
- Design and build a demonstration coal-to-chemicals poly-generation plant in China under the leadership of LP Amina to demonstrate the new poly-generation technology
- Conduct R&D of new coal co-generation systems with CO$_2$ capture, including new approaches for coal-to-chemical co-generation
- Develop advanced gasification catalysts and concepts

Technical Approach

Researchers from both countries are working together to develop new technology to convert conventional power plants into poly-generation plants that make full use of waste heat and oxy-fuel combustion to produce chemicals and further polymers from coal. The approach leverages investments in technology development and industrial implementation aimed at reducing emissions, improving efficiency, and increasing economic benefits associated with coal power production. The technical approach includes the following:

- Build a laboratory-scale research facility
- Develop a new carbothermic reduction process to produce standard industry chemicals from limestone and coal
- Produce synthetic chemicals and fuels
This research will result in the development of a demonstration project at a power plant in Shanxi, China, by LP Amina. In addition to standard engineering analysis, this work will require a substantial amount of basic research, especially in system analysis, reactor dynamics, chemical kinetics, emissions, and process stability and reliability.

Recent Progress
Researchers from the Chinese and U.S. teams have carried out the related R&D efforts smoothly and achieved meaningful progress on co-generation system combined pyrolysis, gasification, and combustion; chemical looping gasification with CO\textsubscript{2} capture; direct synthetic natural gas (SNG) production from coal; gasification properties of the coal direct liquefaction residue; measurement, modeling, and environmental technologies for unconventional coal gasification; and the coal/biomass co-conversion process. Researchers have accomplished the following major achievements:

- Validated coal co-generation technology combined pyrolysis, gasification, and combustion on a 1-megawatt thermal pilot plant; this technology may be demonstrated in industry
- Completed commissioning tests of the constructed ~15 kilograms/hour chemical looping gasification facility and validated the coal chemical looping gasification technology approach
- Obtained coal gas with high-concentration CH\textsubscript{4} from the constructed bench-scale high-pressure constant volume reactor, which validated the possibility of direct SNG production from coal
- Confirmed the feasibility of liquefaction residue for coal gasification and developed suitable additives for coal liquefaction residue and coal mixture slurries
- Utilized a model underground coal gasification test reactor to evaluate the temperature and concentration fields and to draw a model of the cavity
- Developed the key processes and efficient catalyst for co-transformation of biomass and coal based on the constructed experimental platform
- Developed a chemical kinetics model for calcium carbide production, as well as a slag flow model for use with oxy-coal combustion reactor simulations
- Explored effects of temperature and exposure time on the gasification kinetics of Powder River Basin (PRB) coal
- Explored catalytic methods for production of ethylene glycol from coal syngas, including development of a method for catalyst production

Expected Outcomes
The implementation of poly-generation will reduce capital costs, greenhouse gas emissions, and plant maintenance costs of power generation sites. When paired with cleaner coal utilization with increased efficiency and minimal waste, poly-generation will be a cost-effective, commercially viable option for reducing CO\textsubscript{2} emissions in the power generation sector. This approach will also enable minimization of waste heat and/or materials. The LP Amina-Gemeng International Energy plant could reduce greenhouse gases by more than 25% compared to conventional technology. Newly developed catalysts and processes will enable efficient conversion of coal to syngas and related by-products.
Pre-Combustion CO₂ Capture

Research Objective
The development and implementation of the integrated coal gasification combined cycle (IGCC) into power generation is still in the first-of-a-kind stages. In this theme, industrial, research, and academic leaders from both the United States and China will work with industrial-scale demonstration projects and best-in-class technologies to provide the world with robust, transparent cost and performance estimates for IGCC power plants with carbon capture and storage (CCS).

This project has one primary goal: development of techniques to aid in the design and optimization of commercial-scale IGCC systems. Specifically, the team will accomplish the following:

- Assess the economic feasibility and operability of gasification technologies in conjunction with the removal of criteria pollutants
- Assess the technical/economic feasibility and operability of novel carbon capture technologies
- Optimize the economics of different carbon capture technologies
- Establish guidelines/protocols/criteria for system optimization and evaluation, as well as techno-economic analysis and comparison at commercial-scale application

Technical Approach
The project emphasizes system integration, optimization, and key component development. The technical approaches for the project’s two tasks are the following:

Development of techniques for integration and optimization of an IGCC system
- Study the integration, optimization, and modular design of an IGCC system based on the existing research and demonstration experience of the first IGCC plant in China, as well as the experience of both existing and under-construction IGCC in the United States

Understand the key components in a pre-combustion CO₂ capture process
- Design and construct the slipstream-scale pre-combustion CO₂ capture and utilization system by extracting a slip-stream syngas from an existing IGCC plant

To accomplish this work, researchers (led by the China Huaneng Group and assisted by Duke Energy in the United States) will develop techniques for the optimization and design of a commercial-scale IGCC system based on the existing research and demonstration experience of GreenGen, the first IGCC plant in China, and the experience of IGCC at Duke Energy’s Edwardsport Station.

The major obstacles the two companies have been trying to work through include various intellectual property issues and other legal issues with the partners providing the technology.

Researchers (led by Huaneng) will also develop advanced key components, including pre-combustion CO₂ capture featuring heat-integrated, robust, ultrathin barriers with reasonable contamination resistance to flue gas; advanced water-gas shift reactors; advanced separation reagents; and advanced compression technology.

The ACTC team’s specific activities that further pre-combustion CO₂ capture will include the following:

- Developing and fabricating heat-integrated, robust, ultrathin barriers with reasonable contamination resistance to flue gas for both pre- and post-combustion CO₂ removal
• Formulating new CO$_2$ absorbents with chemical additives for pre- and post-combustion CO$_2$ capture with high capacity, fast kinetics, and high stability
• Initializing models for existing pre-combustion capture technologies, chiefly physical sorbents, both as individual models and within the two reference plants (including water-gas shift and gas cleanup)

Recent Progress

Duke Energy’s Edwardsport plant and Huaneng’s GreenGen IGCC reached an agreement on the reporting format and identified that information regarding the following example areas will be exchanged:

- Air separation unit
- Gasification
- Power block
- General utilities and common systems
- Environmental performance
- High-level costs
- Start-up report

Both companies would prefer to hold a workshop at each owner’s IGCC site, as well as to develop a long-term IGCC technology-sharing relationship. There are significant intellectual property issues that will need resolution before a long-term agreement can be developed.

The ACTC team’s specific progress for pre-combustion CO$_2$ capture research includes the following:

• Completed the comparison, selection, and unit modeling of a 30 megawatt thermal (MWth) pre-combustion CO$_2$ capture system
• Completed the process flow diagram, which includes the equipment layout, process equipment tables, major static equipment diagrams, and system control program. Completed the key equipment design of a 30 MWth CO$_2$ capture system based on IGCC
• Completed the capture reagent and process development evaluation. Confirmed the best adsorption temperature and the fittest CO$_2$ concentration of CaCO$_3$ and CaC$_2$O$_4$ as precursors
• The high-temperature, solid-state method is used to modify the adsorbent by doping magnesium, aluminum, cerium, zirconium, and lanthanum. The team found that the adsorption capacity was dependent on different conditions
**Expected Outcomes**

Key outcomes will include critical data, lessons, and knowledge shared through operational experience with demonstration projects as systems are optimized and the cost of pre-combustion CO$_2$ capture is lowered. Such knowledge sharing contributes to accelerating the development of IGCC with CCS, a critical pathway toward low-carbon power generation with coal.
Research Objective

The goal of this task is to integrate advanced capture and solvent technologies into the development of efficient CO₂ capture. Parts or combinations of these technologies will be used to lower the energy costs related to a post-combustion capture process.

The Advanced Coal Technology Consortium (ACTC) team is directly addressing the need for steep emissions reductions from the existing coal fleet by analyzing, testing, and demonstrating technologies for post-combustion capture integrated with sequestration (e.g., storage) at real power plants. Through streamlined bilateral joint cooperation, U.S. and Chinese researchers are looking to accomplish the following:

- Research efficiency improvements for affordable post-combustion CO₂ capture technologies
- Coordinate efforts between U.S. and Chinese partners
- Develop models for post-combustion CO₂ capture, utilization, and storage (CCUS) technology at a commercial scale

Technical Approach

To enable commercial-scale CCUS, the ACTC team is addressing the gap between theoretical energy requirements for post-combustion capture and present-day commercially available technologies. The team’s technical approach includes the following:

- Conduct a pre-engineering study of the 1 million tons/year post-combustion CO₂ capture systems, combined with a preliminary techno-economic analysis and budgetary cost estimate (±30%); upon completion, perform a sensitivity study of power generation with a post-combustion carbon capture system
- Develop innovative solvent compositions to reduce the overall cost of carbon capture and storage (CCS) in three steps: (1) establish a performance matrix for solvent formulation and evaluation, (2) formulate the solvent to balance kinetics and thermodynamics, and (3) conduct evaluations at various levels of scale to determine the solvent’s performance capabilities compared to the matrix
• Use rational design for future catalyst generation, building on the success of previous synthesized mimic catalysts to enhance the CO\textsubscript{2} mass transfer rate in concentrated amine solutions used for post-combustion capture, to demonstrate catalyst stability and robustness under conditions conducive to post-combustion carbon capture, and to demonstrate catalyst performance in a capture process using coal-derived flue gas

• Develop high-throughput CO\textsubscript{2} capture membranes, leading to improved plant efficiency and reduced capture costs via the design and synthesis of highly CO\textsubscript{2}-permselective polyethylene-glycol-based hybrid membrane materials; develop novel methods based on ultrasonically assisted deposition techniques to fabricate ultrathin composite membranes with unprecedented high CO\textsubscript{2} permeances on commercially attractive support platforms; and demonstrate these developed materials and methods via membrane separation evaluations under industrially relevant coal-derived flue gas conditions

• Investigate the use of carbon xerogel and surface-modified carbon xerogel for the enrichment of carbon-loaded monoethanolamine (MEA) and piperazine species using a new flow-through capacitive deionization cell; investigate also integrated cell components with the use of a dc-dc converter to lower overall energy costs

**Recent Progress**

The research team completed the conceptual simulation for a 1 million tons/year post-combustion CCS project in Gibson-3 using technology developed by China Huaneng and demonstrated at the Shanghai Shidongkou Power Plant.

Researchers started a demonstration project at Duke Energy’s Gibson station, where the current cost of CO\textsubscript{2} capture can be effectively evaluated. Catalyst and solvent development will be used to not only prolong the life of the capture solvent, but also to increase mass transfer into the liquid phase, thereby decreasing the size of the absorber necessary in the capture process. The cyclic carbon loadings of the solvent will also be increased through the use of blended solvents.

Researchers have continued development on a two-phase (biphasic) solvent for CO\textsubscript{2} capture. Various biphasic solvents have been screened and analyzed. The work has involved the demonstration of the process using a laboratory-scale absorption/desorption column to yield cyclic capacity for various solvent blend compositions. The separation of the CO\textsubscript{2}-enriched phase resulted in a low circulation rate and reduced the thermal energy requirements for CO\textsubscript{2} desorption. A >30% energy reduction in thermal energy by making use of this biphasic solvent has been projected, although process implications for the separation of these phases would need to be addressed for larger-scale implementation.

The U.S. side has been focused on the development and testing of catalysts capable of withstanding the harsh conditions associated with carbon capture. The work has involved demonstration of a new class of catalyst that can tolerate the high temperatures and flue gas impurities derived from NO\textsubscript{x} and SO\textsubscript{x} gases. Catalyst stability at temperatures up to 140°C and in the presence of flue gas impurities has been established and verified.
A series of candidate catalysts were computationally modeled, guided by previous catalyst results. It was previously concluded, based on computational transition state modeling, that compounds with long Zn–O yet low (<8.5) pKa are needed. Longer Zn–(OH) bonds lead to the following:

- Lower Lewis acidity of the metal-ligand complex
- More of a “free” hydroxide (and more nucleophilic)
- Higher pKa for the H₂O deprotonation step

Researchers completed project objectives for the year, including evaluating catalysts under the more realistic conditions observed in a carbon capture process, high temperatures and flue gas impurities. The newly developed catalysts were able to withstand these harsh conditions and maintain their performance in enhancing the overall mass transfer. Further refining the conclusion from last year based on experimental results, the ligand environment and secondary coordination sphere imparted with our catalysts are key to the robustness of this new class of catalysts.

The U.S. side’s efforts have been additionally focused on the development of hybrid CO₂ separation membranes with high permeability and ultra-thin barrier materials enabling high membrane permeance with improved separation efficiency and decreased separation costs. Ultrathin, ionic liquid-based selective layers of these hybrid materials on commercially attractive supports have been developed with selective layers measuring approximately 100 nm. Reduced crystallinity of the active layer was found to dramatically increase the additive retention of the active layer as well as increase the permeance through the membrane. Production of viable fabrication methodologies for the developed membrane materials has also been examined at larger scale to demonstrate the applicability towards larger-scale processes.

Work on capacitive deionization (CDI) for amine solvent enrichment has focused on long-term cycle operation of moderately scaled-up flow-through capacitive deionization cells as well as integration of a new dc-dc converter for lowering the energy costs of the separation process. Enrichment of carbon-loaded piperazine molecules was shown to reach >10% with current cell designs. Further enrichment will be shown for cells with 10X scale-up planned for Year 5. A new dc-dc converter has shown energy recoveries of >20%, reducing the energy cost of this enrichment process. Further reductions will be necessary to decrease the energy cost further for a beneficial impact in the CO₂ capture process. A third-generation converter is already being planned that will reduce losses of various system components with projected energy recoveries of >30%. Year 5 will demonstrate the use of this new converter towards even lower energy costs.

Figure 3. Flow-through capacitive deionization cell for enrichment of carbon-loaded amine solvents. (a) Schematic of the modular cell and (b) illustrative representation of the solution flow path.
**Expected Outcomes**

All of the research in this project will be used to show that the energy cost of CO$_2$ separation from current power plants and the capital cost of the process equipment can be dramatically decreased. The project will produce optimized design options of competing technology pathways (e.g., advanced solvent) for post-combustion CCUS cost, retrofitability, engineering, and environmental performance. The results from this work will lay the groundwork for decision makers in both China and the United States to understand the potential role of post-combustion retrofits in achieving steep reductions, as well as provide new operational insights into the integration of capture and storage while developing new low-cost, post-combustion capture options.
**Oxy-Combustion CO₂ Capture**

*Research Topic: 5*

**U.S. Research Team Lead**
- Richard Axelbaum, Washington University in St. Louis (acting team lead)
- Kevin McCauley, Babcock & Wilcox Power Generation Group, Inc.

**China Research Team Lead**
- Liu Zhaohui, Huazhong University of Science and Technology

**U.S. Partners**
- Washington University in St. Louis
- Babcock & Wilcox Power Generation Group, Inc.
- West Virginia University
- Lawrence Livermore National Laboratory
- National Energy Technology Laboratory

**China Partners**
- Huazhong University of Science and Technology
- Tsinghua University
- Research Center for Clean Energy and Power, Chinese Academy of Sciences

**Research Objective**

Researchers from the U.S.–China Advanced Coal Technology Consortium (led by the Huazhong University of Science and Technology [HUST] in China and by Babcock & Wilcox [B&W] and Washington University in St. Louis [WUSTL] in the United States) will collect fundamental and pilot-scale data associated with various oxy-combustion conditions and conduct feasibility and economic analysis on the commercial-scale deployment of the technology for CO₂ capture. The objectives for Theme 5 activities are defined as follows:

- Determine combustion and emission characteristics of indigenous Chinese and U.S. coals of different ranks under oxy-combustion conditions
- Evaluate and optimize pilot-scale oxy-combustion technology
- Develop a computational fluid dynamics (CFD) and process model for oxy-combustion
- Enable knowledge sharing on the feasibility study of the large-scale demonstration

**Technical Approach**

With experience from previous U.S. work, along with the development of new research pilots in China, an opportunity exists to accelerate the path to commercialization and broaden the application across regions and fuel types. The primary approach focuses on expanding the experience of oxy-combustion into broader applications in the United States and China. The technical approach comprises five main activities:

**Fuel characterization and hazardous air pollution emission study under oxy-fuel conditions**

- Conduct analysis of representative samples of different ranks of Chinese and U.S. coals
- Conduct experiments on characteristics of coal pyrolysis, ignition, combustion, burn off, dust stratification, slagging, and deposition in bench-scale facilities. Also, conduct tests on NOₓ formation and destruction, PM2.5 emission, and control
- Develop and implement reaction chemistry sub-models on combustion and NOₓ formation under oxy-combustion conditions to provide a tool for burner design and oxygen injection optimization (HUST’s Furnace Model [FURN]) and B&W’s Combustion Model [COMO])

**Pilot-scale oxy-fuel combustion evaluation and optimization**

- Carry out pilot-scale tests in research facilities at B&W and HUST using selected Chinese and U.S. coals
- Configure the research facilities at B&W and HUST for the optimum oxy-combustion flue gas recycling process (e.g., warm-recycle, cool-recycle, or cold-recycle) using a new burner design
- Collect performance data on combustion, heat transfer, furnace exit gas temperature, and emissions over a wide range of practical operating conditions
- Select the most promising design, based on modeling predictions and performance criteria for further demonstration
Steady-state and dynamic process modeling simulations

- Compare Aspen Plus static predictions with pilot-scale data
- Use Aspen Plus Dynamics to simulate transient oxy-combustion processes
- Validate and tune the dynamic process model toward developing a control strategy for start-up, shutdown, modulations, and unit trips (e.g., boiler, air separation unit, and compression and purification unit)

Feasibility study for large-scale deployment

- Facilitate information exchange on policy, investment, and technical issues to conduct a feasibility study of a reference wall-fired pulverized-coal-burning unit for oxy-combustion
- Perform unit and process concept reviews of the air separation unit, boiler island, compression and purification unit, and the balance of plant

Evaluation of novel staged oxy-combustion concept

- Conduct small pilot testing (100–500 kW) under reduced flue gas recycle (increased oxygen concentration) conditions
- Obtain experimental data set for CFD model validation
- Study fly ash and deposition characteristics

Recent Progress

The gas reaction mechanism for oxy-fuel combustion with dry and wet recycle have been developed, and the predictions of gas temperature and composition are more accurate. Based on spectral line-based, a new WSGG model have been developed, which has obvious advantages in non-isothermal and non-homogeneous gas mixture. Predictions of temperature from the HUST CFD model have been compared to experimental data, and good agreement was found.

The characteristics of ash deposits in a CFB were experimentally determined. Oxy-fuel combustion had an obvious influence on the deposition rate, fine particle emissions and the content of S, K, and Na in ash deposits. The effects of sorbent injection (limestone) on deposits were also studied.

Combustion experiments at WUSTL were performed under conditions of increased oxygen concentration. Measurements of temperature, wall heat flux and NOx were taken. This data is being compared against predictions from ANSYS FLUENT CFD model. Model results indicate that heat flux can be controlled in high-oxygen environments by manipulating flame shape and swirl.
An ASPEN process model of HUST’s full chain system (FCS) was developed and an exergy-based optimization method was performed to determine optimal control strategy for flue gas recycle.

**Expected Outcomes**

This project will lead to cost and performance improvements that are rooted in fundamental science from testing in the laboratory and the field. The use of computer simulation and modeling will allow for greater progress on future demonstrations by reducing risk and optimizing both design and critical areas that require large-scale validation. Ultimately, the economic and environmental potential of oxy-firing combustion will be attributable to a wider range of solid fuels and at a commercially viable scale. The use of the computer models, once validated at large-scale commercial projects, will reduce the risk of deployment and increase the speed of deployment for a wide variety of world coals that normally present additional challenges. These small-scale pilots and the computer models will then become a valuable tool for faster deployment of cutting-edge technology in a long-lived, capital-intensive market space.

**Figure 3. China and U.S. research pilots.**

- **FF-EFR (HUST, HIT)**
- **10kW EFR (THU)**
- **3MW Full Chain System**
- **Entrained Flow Reactor**
- **1 MWth Oxy-Combustion**
- **1.8 MWth Oxycoal Pilot**
Research Objective

This theme’s research is focused on identifying utilization targets overlying deep saline reservoirs and integrating carbon capture, utilization, and storage. Target basins include the Ordos and Bohai basins, China, and the Rock Springs Uplift and Illinois Basin in the United States. This effort includes the following:

- Characterize targeted geological storage reservoirs in three dimensions, on both regional and site-specific scales, based on all available public geological, geophysical, geochemical, petrophysical, petrographic, and petroleum engineering data. This research is especially concerned with characterizing reservoir and seal heterogeneity, as well as the effects of heterogeneity on CO$_2$ injectivity and storage capacity assessments.
- Develop the scientific, technological, and engineering framework required for CO$_2$ utilization in the Illinois and Ordos basins via enhanced oil recovery (EOR), shale gas, and enhanced coal bed methane (ECBM). Utilization in the Bohai Basin (Tianjin) includes enhanced water recovery (EWR) and couples to capture at the Huaneng GreenGen IGCC facility. The utilization strategy will include safe, permanent storage of large quantities of anthropogenic CO$_2$.
- Develop simulation technology for CO$_2$ storage in saline formations.
- Research and apply monitoring technology of CO$_2$ storage in saline formations.
- Assess safety and risk of CO$_2$ storage in saline formations.
- Understand system feedbacks, including the impacts of source locations on optimization of storage systems.
- Conduct geological characterization at multiple data resolutions.

Through combined research on these issues and successful execution of demonstration projects, this effort will improve understanding, provide verification of key technologies for CO$_2$ storage in saline formations, and provide the scientific evidence to implement large-scale CCS and CCUS in China and the United States.

The project has two primary objectives:

- Build the scientific, technological, and engineering framework necessary for CO$_2$ utilization through EOR and EWR, and the safe, permanent storage of commercial quantities of anthropogenic CO$_2$ in geologic formations in both China and the United States.
- Assess the safety and risk of CO$_2$ storage in saline formations.
**Technical Approach**

In the near term (2014), the team plans to accelerate data collection and move forward with work in Ordos and Bohai Bay basins (China), the Illinois Basin, and the Green River Basin (Rock Springs Uplift) in Wyoming. Both the United States and China are working to determine what data can be released publicly to facilitate collaboration that will allow use of the best algorithms from both China and the United States. The team continues to monitor the progress of developments in the coal-to-liquid industry in the Ordos Basin as sources of lower-cost CO$_2$ for EOR.

Collaboration at the site scale requires application-dependent cooperation that may or may not involve direct sharing of sensitive data. Sharing executable algorithms will allow teams on either side to create results using the range of tools available to the U.S.–China Clean Energy Research Center (CERC). The team will continue to pursue opportunities to exchange personnel to increase productivity and joint understanding of algorithm implementation. Both U.S. and Chinese teams continue to develop models for specific sites in their own countries that will support the overall goals of the project without constraints. Specifically, using the University of Wyoming projects as analogs, the team proposes to work closely with research scientists from the Shaanxi Provincial Institute of Energy Resources and Chemical Engineering and Northwest University to assess the anthropogenic CO$_2$ resources and geological CO$_2$ storage capacity of the Ordos Basin.

Methods employed in a comprehensive regional storage analysis include coupling impacts related to the reality of multiple sources linked to multiple possible sinks including all relevant sources of uncertainty. Such regional studies allow intelligent development of both capture systems and storage sites based on evolving CO$_2$ capture goals. Algorithms developed at LANL over the past several years are being driven by detailed data on CO$_2$ sources, utilization targets, surface features (mountains, rivers, cities, etc.), and estimates of both storage capacity and injectivity for specific reservoirs. We are using the approaches developed in our previous work with new modifications to tackle ECBM/Shale Gas/EOR/Saline CO$_2$ storage questions associated with the Gibson/southern Indiana region and plan to teach/demonstrate the same techniques to our collaborators from the Chinese Academy of Science and Northwestern University.

**Recent Progress**

The Yangchang Oil Company has initiated a CO$_2$ storage and CO$_2$–EOR project, and injection of CO$_2$ was successful (Figure 1). Company representatives visited Wyoming to seek assistance with project design (e.g., reservoir heterogeneity characterization, structural and property modeling, injection and production simulation, economic evaluation). The joint project team arranged a joint field trip in the Ordos Basin to study the targeted storage reservoirs and potential sealing strata, and to observe cores in the Yanchang and North China Oil Company core repository. To assist the Yanchang Oil Company with its CO$_2$–EOR and storage demonstration projects, the team organized a trip to work on the reservoir data at the Yanchang facility in order to continue to build structural and property models.
A visit to Los Alamos National Laboratory in September 2013 by Dr. Bai of the Chinese Academy of Sciences led to data sharing on sources of CO$_2$ located around the Ordos Basin. This data sharing allowed us to create a source/sink model of what large-scale (50–300 MT/yr) CCS might look like in the future (Figure 2). This work was presented at GHGT-12 in Austin, October 2014. A workshop in May 2014 in Wuhan brought together many of the primary researchers, and progress was made in determining how to proceed with generating regional-scale data from publicly available sources that can be shared between both countries. Additionally, initial work in the Illinois Basin on stacked CO$_2$ utilization with deeper large saline reservoirs for a range of CO$_2$ capture (1–15 MT/yr) was presented to Duke Energy, and a report is being generated based on suggestions from the presentation.

Using these models, the team will perform, at facilities in Wyoming, numerical simulations for the targeted reservoir and storage site. Detailed three-dimensional geological, structural, and property models are being constructed for the selected mature oil reservoir (i.e., targeted CO$_2$ flooding reservoir). Reservoir heterogeneity will be built into these models using outcrop and core observations, well log analyses, seismic interpretations, and Wyoming analogs (Figure 3).

In the last year, the partners from Northwest University, Shaanxi Provincial Institute of Energy Resources and Chemical Engineering, the Yanchang Petroleum Company, the North China Oil Company, the Institute of Rock and Soil Mechanics, China University of Mining and Technology, the University of Wyoming, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, the Indiana Geological Survey, and West Virginia University have accomplished the following tasks:

- Assembled a large set of information regarding the geologic, petrophysical structural/stratigraphic frameworks of the Ordos Basin, Rock Springs Uplift, and Illinois Basin
- Inventoried the distribution of fossil energy and anthropogenic CO$_2$ resources in the Ordos Basin
- Delineated CO$_2$ sources, sinks, and utilization targets in the Illinois and Ordos basins in a presentation to Duke Energy
- Delineated CO$_2$ sources for Wyoming
- Explored the potential of developing CCUS analogs between the Ordos Basin and the Powder River/Green River Basin and Illinois Basin using the latest screening criteria
- Published results from a numerical study of CO$_2$ injectivity, storage capacity, and leakage for the Rock Springs Uplift in Wyoming in the *International Journal of Greenhouse Gas Control* (impact factor [IF] 5)
- Published results from an analysis of the impacts of CO$_2$ source variability on storage costs in *Applied Energy* (IF 5)
- Published source sink matching work in the Ordos Basin (*Energy Procedia*, Figure 2)
- Published a methodology for regional-scale system analysis using data from the southeast United States in *Energy & Environmental Science* (IF 15, Figure 4); methodology adapted partially from the National Risk Assessment Partnership (NRAP) and applied to the Gibson site to emulate multiphase flow and reactive transport
- Published work on a path forward in the United States for CCUS using high-value chemicals (*Energy Procedia*)
- Published in *Environmental Science and Technology* on how utilization and CO$_2$ sources are not well matched (IF 5)
• Developed site prioritization methods and ranked saline storage reservoirs
• Leveraged collaboration between the Yangchang Oil Company and the Theme 6 team to initiate design, construction, and injection at a pilot CO₂–EOR project in the Ordos Basin
• Delivered a 70-page pre-feasibility study on EWR coupled to CO₂ capture at the GreenGen facility to the Huaneng Group

**Expected Outcomes**

The significant opportunity for storage and utilization of CO₂ in the Ordos Basin in China complements opportunities that are being explored in basins in the United States, such as in Wyoming and Illinois. The research team is looking at the Ordos Basin in parallel to this research. The lessons learned will be invaluable to CCS projects, particularly in Rocky Mountain basins; the Majiagou Limestone and Ordos Basin are very similar to the Paleozoic Madison Limestone and the Powder River Basin of Wyoming and Montana.

This work ultimately improves global understanding of how to safely and effectively store CO₂ in saline formations or to use the CO₂ for EOR.

The most important outcomes expected at the end of Year 5 are as follows:

• Jointly developed structural, property, and numerical models (including the heterogeneity of the reservoir/seal system) for the highest-priority geological CO₂ storage reservoirs and sites in the Ordos, Green River, and Illinois basins
• A detailed evaluation of all anthropogenic CO₂ sources and sinks in the Ordos, Green River, and Illinois basins
• Initial optimization strategies for pipeline networks in the same basins considering utilization targets such as EOR, EWR, ECBM, and shale gas co-located with deeper saline storage reservoirs.
• A demonstration project, developed in cooperation with Theme 6 partners, to evaluate the potential of integrated geological CO₂ storage with EOR and/or EWR using CO₂ flooding
• A Phase 2 feasibility study for the GreenGen EWR project in Tianjin, China
CO₂ Utilization
Research Topic: 7

U.S. Research Team Lead
- Mark Crocker, University of Kentucky

U.S. Partners
- University of Kentucky
- Duke Energy
- National Energy Technology Laboratory
- Pacific Northwest National Laboratory

China Research Team Lead
- Zhenqi Zhu, ENN Group

China Partners
- ENN (XinAo Group)
- Zhejiang University
- Jinan University

Research Objective
The objectives of this project are to develop and demonstrate an economically feasible technology for CO₂ utilization with microalgae and to transform algal biomass into a sustainable source of energy.

This project aims to accomplish the following sequential goals:
- Identify and culture optimal summer and winter algae strains to be used in the CO₂ mitigation system
- Optimize the culturing process and technology; this should include a demonstration of algae cultivation at pilot-plant scale under summer and winter conditions, incorporating optimized nutrient and water recycling
- Identify and evaluate the possible co-products from the process, including fuels and animal feed
- Use the data gained to construct a techno-economic model to estimate the overall cost of CO₂ fixation and utilization at various scales of operation

Technical Approach
The work plan is divided into four main tasks: screening algae strains; optimizing the growth system; developing efficient, cost-effective post-processing technologies; and conducting techno-economic analysis. The ongoing tasks include the following:
- Optimize the gene transformation method
- Optimize water recycling
- Optimize nutrient recycling; for example, from anaerobic digestion of harvested algae
- Demonstrate winter operation
- Develop an efficient and effective extraction technology suited for the selected algal species
- Develop a cost-competitive harvesting and dewatering technology with minimal process energy intensity
- Evaluate anaerobic digestion of algae for biogas production
- Conduct economic analysis of the possible power plant savings and costs associated with CO₂ utilization by microalgae

Recent Progress
Large-scale carbon fixation using microalgae was conducted at ENN’s demonstration facility, located in Inner Mongolia. The carbon source was from a coal gasification plant, co-located with the cultivation facility. Through optimization of cultivation and effective contamination control, the pond (1,200 m²) was run for 70 days continuously without contamination disruptions. The average productivity reached 20 g/m²/d, including rainy days. In addition, the supernatant from harvesting was treated and recycled during the cultivation trial.

A subcritical wet algae extraction technology was developed, optimized, and tested at small scale with capacity reaching 10 kg/d and the oil recovery rate exceeding 90%. The current estimated cost for processing one metric tons of oil was 3,300 Yuan. In addition, a successful separation for defatted biomass, water, and solvent was achieved, with a solvent recovery rate exceeding 74%.
Research efforts at East Bend Station were focused on the operation, and expansion, of the photobioreactor system (Figure 1). Biomass productivity was correlated with weather conditions such as temperature and available sunlight (photosynthetically active radiation or PAR). A techno-economic analysis was performed using the cost and performance data from the pilot-scale system. This analysis revealed the most important factors that drive the costs associated with the beneficial re-use of carbon dioxide using microalgae and informed where improvements needed to be made. Factors such as amortization period, capital cost of PBR, and potential utilization pathways were considered and improved.

One example of the benefit of this analysis showed that two of the biggest costs associated with the current PBR design were the frame and control system. The team at the University of Kentucky (UK) engaged the departments of Mechanical Engineering (ME) and Electrical Engineering (EE) to use senior design projects to produce more cost-effective approaches. The ME team reduced the cost of the frame by 67% and the EE team reduced the costs associated with the control system by more than 80%. Both of these designs were rolled into an updated PBR design that made more efficient use of capital by changing the way the system was laid out and operated. By implementing a staggered tube design operated in cyclic flow mode, the capital cost was reduced, the productivity was increased, and energy consumption was minimized, greatly improving the overall economics.

Another major effort focused on the evaluation of using anaerobic digestion to produce a “bio-gas” as a potential utilization pathway for the produced algae biomass. Harvested algal slurry was subjected to a variety of pre-treatments and fed to a batch anaerobic digester, and parameters were measured such as volatile solids, produced bio-gas constituents, and the composition of the digestate waste from the process. Promising results showed 50% of the digestate was suitable for immediate recycle to provide nutrients to support the cultivation step. The remaining solids could be processed
for nutrient recycle or sold as a soil amendment based on further analysis. A life cycle analysis of the whole CO₂→algae→AD→Biogas pathway is currently underway to determine greenhouse gas reduction potential.

Support efforts at UK have focused on evaluation/characterization of a promising winter strain (*Chloromonas sp.*), continuing the development of a low-cost/low-energy dewatering process, and the creation of methods to evaluate the biomass composition (protein/carbohydrate/lipids) to better inform potential utilization strategies.

**Expected Outcomes**

Process data (CO₂ capture efficiency, areal biomass productivity, energy consumption, nutrient consumption, etc.) of the new system will be collected at the East Bend pilot installation throughout the second and third quarters of 2015. Large-scale carbon fixation growth studies will be continued at the demonstration facility in Inner Mongolia. Accumulated data will be incorporated in an updated techno-economic model that will enable the costs associated with CO₂ capture and utilization to be calculated at different operating scales.

Efforts will continue to develop the collaborations between the U.S. and Chinese partners. Initial data sharing has already taken place regarding the research efforts of both ENN and UK at East Bend station. The 2014 CERC-ACTC meeting in Hangzhou was very productive in enhancing collaborative opportunities. The UK team met with new ENN researcher Dr. Xuemei Bai and Professor Dr. Jun Cheng from Zhejiang University (Figure 4). Discussions have begun between Zhejiang University, ENN, and UK regarding expansion of the techno-economic analysis to include cost and performance data from multiple locations. Data sharing between the different partners will enable a range of process configurations and environmental considerations to be assessed (e.g., open-pond cultivation systems versus closed-loop photobioreactors).
Simulation and Assessment

Research Objective

The objectives for this project are to apply modeling techniques to a wide variety of issues associated with pre- and post-combustion CO\(_2\) capture and oxy-combustion in order to accomplish the following:

- Assess the economic and operability potential of existing capture technologies in conjunction with the removal of criteria pollutants
- Assess the technical feasibility and potential economic benefit and operability of novel carbon capture technologies
- Optimize the economics of different carbon capture technologies

Technical Approach

On the U.S. side, three main subtasks have been identified:

Power plant cycling and load-following operation

This is a new task, and the U.S. Department of Energy’s (DOE’s) National Energy Technology Laboratory is focused on determining the effect that power plant cycling and load following have on the life and maintenance of the plant, and how improved strategies can be implemented to prolong the life and reduce the maintenance needed for these facilities.

Systems modeling of post-combustion capture technology

This task involves plant-wide steady-state and dynamic modeling of multiple trains of CO\(_2\) capture equipment. It is focused on the steady-state and dynamic simulation of post-combustion carbon capture processes. The major focus of this part of the work will be to formulate optimal control strategies for multi-train, amine-based processes faced with process disturbances and changes in base loading.

Initialization of dynamic model with immersive visualization

This task involves implementation of a three-dimensional (3D) immersive training system for an integrated coal gasification combined cycle (IGCC) operator training system. It is focused on upgrading the facilities at the West Virginia University (WVU) Advanced Virtual Energy Simulation Training and Research (AVESTAR) Center to provide full 3D immersive training capabilities for the IGCC operator training simulator. The purpose of this work is to develop training materials to enable industry and universities to have a better understanding of coal-based carbon capture power generating systems.

Recent Progress

Researchers simulated a steady-state base case based on Cost and Performance Baseline for Fossil Energy Power Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity (November 2010, DOE). The simulation was based on the monoethanol amine (MEA) solvent case for CO\(_2\) capture from a supercritical pulverized coal power plant. A converged steady-state solution (Aspen Plus) was obtained, and then a parametric optimization was applied; the net result of this optimization was a reduction in the energy penalty from 12.7 to 10.2 percentage points and a
resulting value of 3.07 gigajoules/ton for the heat duty per ton of CO₂ recovered. This optimized case was used as
the starting point to generate a pressure-driven dynamic model using Aspen Plus Dynamics. Researchers converged
the dynamic model, and the steady-state results compared well with the results from the dynamic simulation. A
presentation covering the results of this work was made at the annual American Institute of Chemical Engineers
meeting in Pittsburgh.

More recently, a full dynamic model of multiple parallel absorber/stripper units for the capture of CO₂ using MEA
has been created. Both the efficiency of capture and the pressure drop through the equipment have been
accurately modeled using customized scripts in Aspen Plus Dynamics. The response of the system to changes in flue
gas flow rate and composition has been investigated using standard PID and linear Model Predictive Control (MPC)
schemes. The MPC method provides superior control and adjusts each train of absorption and stripping separately
to obtain the optimum capture rate. Full system identification is underway, and investigation of other control
techniques such as non-linear MPC and robust control will be investigated in the future.

The software licenses and all necessary hardware for post-combustion capture system modeling were specified and
purchased for the implementation of the 3D immersive training system at WVU. The hardware was successfully
connected, and the system was commissioned and is operational. The EYESIM™ software and hardware platforms
were updated recently to make use of high-speed video boards and advances in image processing.

Research has been conducted in the area of retrofitting power plants with carbon capture. A study was conducted
on performance changes of a steam turbine with stream extraction for a carbon capture unit using accurate
modeling tools provided by a steam turbine manufacturer. The relationship between the power output of a steam
turbine, the flow rate of the main steam, and the amount of steam extraction was developed. Finally, the
relationship was identified between the pressure of the extracted steam and its flow rate, and the flow rate of the
main steam, combined with minimum extraction pressure and maximum flow speed constraints.

A dynamic model was developed of a single train of an industrial-scaled carbon capture unit, based on the model of
a pilot unit, and the dynamics of a carbon capture unit and steam turbine under load changes were analyzed.

The team also conducted a performance comparison of IGCC plants with ion transport membrane (ITM) air
separation and cryogenic air separation. Comparison results show that an IGCC plant with ITM air separation is
superior on all fronts to an IGCC plant with cryogenic air separation. Increasing the integration degree and high-
temperature nitrogen re-injection can lead to even higher energy efficiency.

Researchers developed modular models of key functional blocks for IGCC plants. Modular models for coal
gasification, air separation, sulphur removal, and combined cycle were developed with consideration of integration
between these units. A CaO-based CO₂ capture process was integrated with the coal gasification process in a single
reactor. The unconverted char from the process provided the heat required to regenerate the CaO.

**Expected Outcomes**

Application of advanced modeling and simulation tools—e.g., dynamic simulation and H∞ control—will enable
improvements in technology and systems integration that would not otherwise be possible, because of the very
complex nature of the interacting processes present in large-scale power generators with carbon capture. Such
improvements will decrease the cost and improve the performance of CO₂ capture technologies by providing a
platform on which different process control schemes can be demonstrated and optimized prior to their
implementation in CO₂ capture processes.