Quarterly Progress Report

January 1 – March 31, 2014

Cooperative Agreement DE-PI0000017

West Virginia University Research Corporation

US-China Clean Energy Research Center
Advanced Coal Technology Collaboration

Project Director & Principal Investigator: Jerald J. Fletcher

Phone: 304-293-5499

Fax: 304-293-3752

Email: JJFletcher@mail.wvu.edu

Quarterly Progress Report

January 1 – March 31, 2014

Executive Summary

The project supports collaborative activities of the US Advanced Coal Technology Consortium (ACTC) as part of the US-China Clean Energy Research Center (CERC) during the second quarter of the fourth project year – January 1, 2014 through March 31, 2014.

During the current reporting quarter, the CERC-ACTC team worked to develop a joint annual technical report in conjunction with our Chinese partners. Researchers from both teams and industrial partners contributed to the development of this report. Other activities included a technical meeting with the DOE Fossil Energy technology team at the National Energy Technology Laboratory, to discuss the work ongoing and planned in the CERC-ACTC, and how this aligns or could better support work currently in the DOE Fossil Energy/Coal research portfolio.

The project team continues to await a written review and comments from the Executive Committee pursuant to the review meeting held in Washington DC in July 2013. Overall response and feedback on the project activities and structure was positive at both the Washington and Jackson meetings, and the team will work to address and implement feedback from the DOE upon receipt.

The CERC-ACTC project has decided to seek the appointment of a full time project director, to consolidate the directorship of the project. This activity is on-going.

*Reporting Note: Owing to requests from the DOE, the report is organized differently than previous reports. Theme 0 (Adminstrative) has been moved to the rear of the report, with the report now beginning with Theme 1.

Quarterly Progress Report

January 1 – March 31, 2014

Project Performance

This report summarizes the collaborative activities of the US Advanced Coal Technology Consortium (US ACTC) as part of the US-China Clean Energy Research Center (CERC) supported by the US Department of Energy (DOE) under Cooperative Agreement DE-PI0000017 (US-China Clean Energy Research Center, Advanced Coal Technology Collaboration) with the West Virginia University Research Corporation (WVURC) during the second quarter of the fourth year of the project (January 1 through March 31, 2014).

The project is composed of a project management theme, eight research themes and an international integration, communication and intellectual property theme:

Theme 0—Project Management Activities
Theme 1—Advanced Power Generation
Theme 2—Clean Coal Conversion Technology
Theme 3—Pre-Combustion CO_2 Capture
Theme 4—Post-Combustion CO_2 Capture
Theme 5—Oxy-Combustion CO_2 Capture
Theme 6—CO_2 Sequestration Capacity and Near-Term Opportunities
Theme 7—CO_2 Algae Biofixation and Use
Theme 8—Integrated Industrial Process Modeling and Additional Topics
Theme 9—Communication, Integration and Intellectual Property Rights Management

This report outlines the approach taken, including specific actions by subtask. If there was no identified activity during the reporting period, the appropriate section is included but without additional information.

Theme 1 – Advanced Power Generation

Subtask 1.1. – Increase efficiency and availability of Existing Coal-Fired Power Plants

Approach

1. Survey existing population of coal-fired power plant sizes and types that offer the greatest opportunity for improvement in China and the US.
2. Identify specific units in both China and the US, with similar characteristics, and conduct a bench-marking study on best operating practices and designs.
3. Investigate specific needs due to cycling.
4. Evaluate other potential improvements based on the state of the art designs being deployed today.
5. Provide final toolbox of improvements that can be used by either China or the US to improve operations.
6. Conduct a workshop to present results and get additional feedback.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

There are no joint plans for the upcoming quarter. Tsinghua and Shanghai Jiaotong are independently pursuing continued work on the following topics:

1. Use online monitoring and operation data to improve performance
2. Reduce power consumption of the balanced draft system

Subtask 1.2. – Advanced Ultra-Supercritical Boiler (A-USC) Development

Approach

Research on 600MW USC boiler of 700℃ main steam temperature combusting Xinjiang coal from Houxun coal field, provide technical support for power generation using Houxun coal efficiently with low pollution.

1. Research on thermodynamic system of 700℃ USC units combusting Xinjiang coal.
2. Design scheme of 700℃ USC boilers combusting Xinjiang coal.
3. Research on coupling characteristics of combusting and hydrodynamics of 700℃ USC boilers.
4. Research on fouling and slagging characteristics of 700℃ USC boilers.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

There are no joint plans for the upcoming quarter.

Subtask 1.3 – Optimize pulverizing system for subcritical power plants with a focus on NOx control

Approach

The technical approach to determining the impact of such retrofit efficiency technologies as the LP Amina static classifier is as follows:

1. Evaluate the current state of installed coal-fired plants in China and the US with regards to pulverizer upgrades and the potential for efficiency and performance improvements. This study should include evaluating different types of pulverizers and milling systems to facilitate development of a target project strategy.
2. Collect and analyze data on classifier installations (LP Amina's A-type)
3. Model effect of staged fineness on NOx reduction, soot formation, ash fouling, slag, etc. (incl. China Zhundong coal)
4. Develop validated models for prediction of particle segregation / separation in cyclone separators.

Based on items 2) & 3) above, develop a technical paper that discusses how improved fineness can be used to improve boiler performance and lower NOx (may need to be staged, coupled with LNB + OFA system, etc).

Based on item 1) above, identify target projects in both China and the US where these new classifiers can be installed on all the mills on a large coal-fired unit so that the predicted benefits for UBC, NOx emissions, unit turndown, and fuel flexibility can be evaluated on a unit basis where all mill classifiers have been upgraded.

Results and Discussion

LP Amina has returned to the laboratory over the last quarter to better understand the fundamental physics behind dense particle flow. A scaled-down version of LP Amina's static classifier has been built in a lab north of Beijing. Additionally, LP Amina is working with West Virginia University to improve its modeling capabilities using ANSYS.

Tsinghua University is designing a new type of low NOx burner for super- and ultra-supercritical wall-fired boilers (600 MW and above) to meet the new emissions standards to which Beijing, Shanghai, and Guangzhou are being held. They are hoping to model the effect of fineness on boiler performance this summer, and perform a demonstration project on a wall-fired unit in China this fall.

Plans for Upcoming Quarter

LP Amina plans to tune its models so that the results match the experimental data more closely. Once a better understanding of the fundamentals is obtained, further improvements of existing installed classifers can be pushed forward. THU plans to continue its modeling work on the new burner and measure the impacts of fineness on burner performance.

Theme 2 – Clean Coal Conversion Technology

Subtask 2.1. – Co-Generation System with Combined Pyrolysis, Gasification, and Combustion

Approach

There has been significant progress in all different fronts: reactor model, experiments, and simulations. Concerning the reactor model, a literature review was performed to understand the formation of calcium carbide from burnt lime in multiphase reactions. The models and experiments performed by several authors were carefully studied. The intermediate reactions required to form calcium carbide from burn lime were investigated and used to formulate our own model. The kinetics of the overall reaction was also studied and a method to obtain the parameters of Arrhenius reaction rates from these experimental results was developed. Some preliminary calculations were done using some of the Arrhenius parameters found in the literature with a perfectly stirred reactor model, and the results compared to experimental data. The energy equations for the overall batch reactor to produce calcium carbide, as well as for each phase present in this reactor, were derived.

The melting temperatures of the main species in the calcium carbide reactor, and in the flue gas and ash/slag of the heat provider oxy-coal combustor were investigated. Their combination in binary, ternary and quaternary phase diagrams was also researched to study ways of decreasing the temperature and time required in the calcium carbide reactor. A combined model of the oxy-coal combustor and calcium carbide reactor is under development.

In the experimental work, cylindrical shape pellets were made from calcium oxide and carbon graphite to study initial reactions in a 4 ft long tube furnace. These experiments were run for a duration of 60 min at 1000 and 1500ºC. Additionally, the microwave furnace power is being increased to 12kW in order to reach the desired temperature levels.

Numerical simulations of the 100kW oxy-coal combustor have been continued and the effect of the percentage of oxygen in air and the swirl profile in the primary inlet on the flame and the temperature profiles near the burner has been investigated.

Results and Discussion

Reactor Design

The preliminary design of the WVU Very High Temperature Entrained Reactor (VHTER) has been completed, including implementation of safety features designed to allow for safely shutting down the reactor in the case of internal pressure increases resulting from blockage of gas exhaust outlets. Efforts are currently underway to complete a thermal stress analysis of the reactor, as well as to generate engineering drawings for use in manufacturing.

CFD Simulations

New simulations are currently being conducted for the purpose of verification and validation of the Reduced Order Model (ROM). These new simulations are based upon the VHTER reactor design and will be used to provide additional reactor exhaust gas temperature and composition data. This additional data will allow for the development of correction factors to be used in the ROM model. These correction factors are necessary due to the assumption of chemical equilibrium inherent in the NASA CEA (chemical equilibrium with applications) code utilized by the ROM model. A journal paper is currently being prepared based upon this effort, and will be submitted for publication at a later date.

Simulations have been conducted in support of the efforts of our industrial partners (namely L P Amina) in the development of their CTC horizontal reactor and the results of those simulations have been provided to them.

Future Work

Over the next quarter, additional CFD simulations will be conducted as needed.

Carbothermic Reaction in Oxy-Combustion

The MSR model detailed in previous reports is currently being modified for use in conjunction with the "slag flow" model currently under development.

Furnace Experiments for Determining Kinetic Rates

Analysis of data collected during the previously reported experiments has continued. For each of the experiments conducted, percentage weight loss, percentage lime consumption, and percentage of calcium carbide remaining in the final samples have been determined. Figure 2.1.1 shows the recorded weight loss as a function of temperature and pellet residence time. In general, the data shows increases trends with temperature and residence time, as to be expected. In addition, the initial weight loss at time = 0 minutes is due to the effects of the slow heating rate required within the conventional tube furnace. Previous research have shown that the carbide reaction can take place at temperatures as low as 1400°C, therefore, some reactions will occur prior to the tube furnace reaching the desired temperatures, if those temperatures are higher.

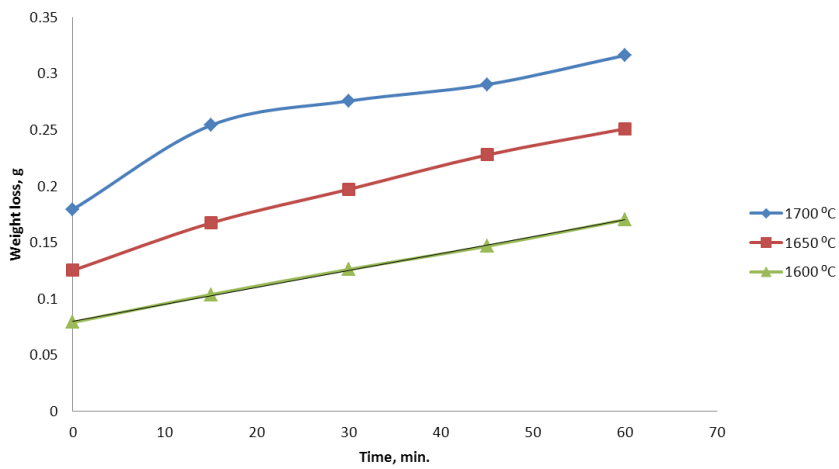

Figure 2.1.1: Weight loss as a function of temperature and residence time in tube furnace.

Please note that the student conducting these experiments completed the requirements for his Master's degree during this reporting period and will be graduating shortly. A postdoctoral fellow has been hired to continue the experimental work, but will need some time to get up to speed. The initial tasks for this new postdoctoral fellow will be to repeat a small number of the previous student's experiments in order to establish a baseline before conducting new ones.

Future Work

As mentioned above, a new postdoctoral fellow has been hired to conduct further calcium carbide formation experiments in both the tube and microwave furnaces. A preliminary test matrix has been generated that will begin to explore the effects of changing carbon monoxide partial pressures within the furnace on the reaction kinetics. Additional experiments to examine

the effects of different carbon sources, as well as differences between using pelletized and loose powder carbon/lime mixtures. The results of these experiments will be used to refine the kinetics data used in the multi-step reaction model discussed previously.

Plans for Upcoming Quarter

No input.

Subtask 2.2. – Chemical Looping Gasification With CO_2 Capture.

Approach

The proposed chemical looping gasification process using CaO as a CO_2 acceptor may obtain high hydrogen content gas from the gasifier while the CO_2 rich gas will be produced using a little pure oxygen in the combustor.

Results and Discussion

No activity this quarter.

Plans for Upcoming Quarter

No input.

Subtask 2.3. – Direct SNG Production from Coal

Approach

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 2.4. – Coal to SNG by Catalytic Gasification

Approach

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 2.5. – Gasification Properties of Coal DTL Residue

Approach

The Shenhua Direct Coal Liquefaction (DCL) process produces petroleum-like fuels by direct hydrogenation of coal. The unconverted coal fraction (residue) can be gasified to produce

hydrogen for the process or syngas for conversion to additional products. Coal can be added to the gasifier feed to increase the quantity of hydrogen or syngas.

If this process were to be built in the U.S., there is a high probability that it would use Powder River Basin (PRB) coal. To identify appropriate gasifier technology for the residue derived from PRB coal, we are pursuing a two part experimental strategy. The first part is to measure the gasification kinetics of PRB coal under conditions that simulate a fluidized bed gasifier. The second part is to solvent extract PRB coal with tetralin under elevated temperature and pressure. We will carry out additional gasification kinetics experiments with the residue of this extraction, which should be similar to the DCL residue.

PRB coal is a benchmark coal for gasification technology. PRB coal, and more reactive feedstocks such as lignites and biomass, give good yields in fluidized bed gasfiers. Coals with lower reactivities do not give good yields in fluidized bed gasifiers, and higher temperature, entrained flow gasifiers are recommended for these coals.

If the residue is more reactive than PRB coal, then a fluidized bed gasifier will be recommended. The residue will have a high mineral content due to the disposable liquefaction catalyst and due to the concentration of ash. Since fluidized bed gasifiers operate under non-slagging conditions, the heat of melting this mineral content can be avoided. There is also the possibility that the catalyst can be separated from the ash and recycled. If the residue is less reactive than the parent PRB coal, then an entrained flow gasifier will be recommended.

Results and Discussion

PRB gasification rates in CO_2 were measured over a 1 to 12 atm pressure range and an 833 to 975 C temperature range. The coal extraction apparatus is under construction.

Plans for Upcoming Quarter

The CO_2 gasification data is being analyzed and prepared for publication. PRB gasification rates in steam will be measured. We intend to complete the coal extraction apparatus and initiate coal extraction experiments.

<u>Subtask 2.6. – Measurement, Modeling and Environmental Technologies for Unconventional Coal Gasification</u>

Approach

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

<u>Subtask 2.7. – Coal/Biomass Co-Conversion Processes</u>

Approach

Gas chromatographic analysis was done for two purge gas feed rates (i.e., nitrogen 100 and 200 sccm) in WVU pyrolysis unit. Additionally, two types of tests have been conducted using the Enerac exhaust analyzer. The first type is to heat the reactor chamber to a given temperature and

taking a sample with the analyzer. The second type is to sample with the analyzer every 100ºC. Both tests were done for 10 g. of coal with a purge gas flow rate of 200 sccm. The product yields are being monitored and analyzed.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 2.8. – Coal to Chemical Production of Ethylene Glycol

Approach

Syngas to ethylene glycol contains two main steps: (1) reaction of CO with ethyl nitrite (EN) to form diethyl oxalate (DEO) and (2) hydrogenation of DMO to ethylene glycol. To achieve the first step, the experimental set-up used for synthesis of EN was built and its schematic drawing is shown in Figure 2.8.1. Three-necked bottled was fixed on an iron stand with a flask clamp. Water bath container and stirrer were put under the bottle. Thermometer, constant pressure funnel and condenser were connected with the bottle. All the connectors were sealed with wax followed by Parafilm. Vacuum tubing was used to connect the condenser with the filtering flask (#7) which was filled with DI water to remove the methanol from the gas. Flask (#7) was then connected with the buffer flask (#8) by vacuum tubing and flask (#9) was connected orderly. Flask (#9) was filled with concentrated sulfuric acid (98%) to remove the moisture from the gas. All the flasks were fixed with clamps and sealed with rubber stoppers. Rubber stops were further sealed with wax followed by Parafilm. Flask (#9) was then connected with two drying tubes (#10) which were filled with anhydrous calcium sulfate to further remove the moisture from the gas. The heads of drying tube were further sealed with wax followed by Parafilm. Drying tubes (#11) were then connected the regulator (#17) of methyl nitrite cylinder via vacuum tubing and a three-way valve (#12). One head of the valve was connected to either oil pump (#13) or the regulator (#14) of the nitrogen cylinder. Oil pump (#13) and the regulator of nitrogen (#14) cylinder were connected with the three-way valve (#12).

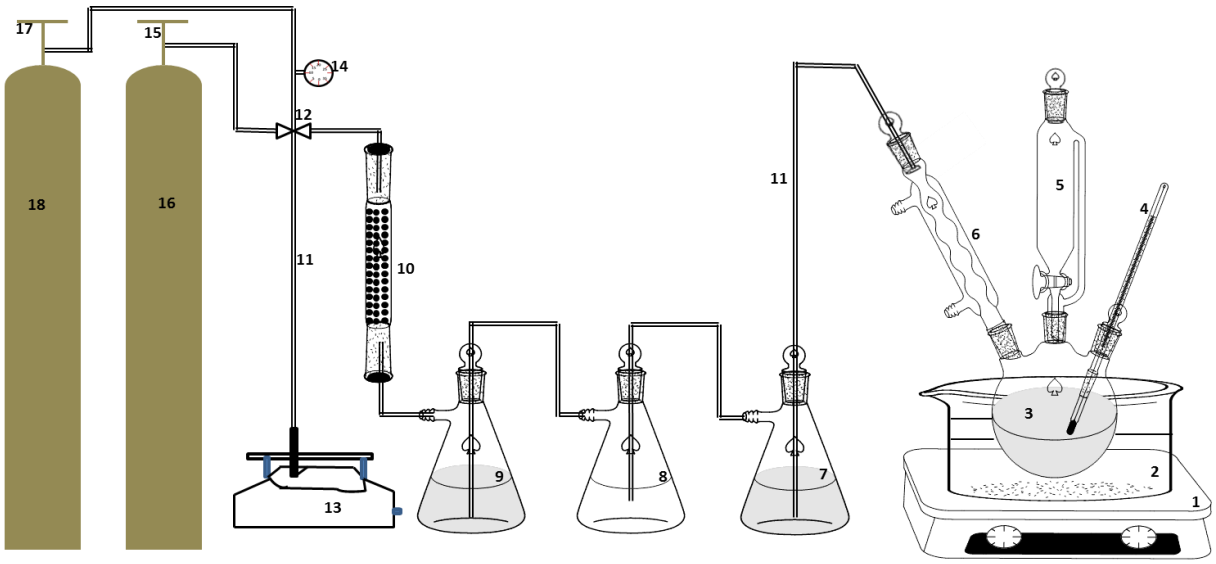

Figure 2.8.1. The experimental set-up of ethyl nitrite production. 1. Stirrer; 2. Water bath container; 3. Three-necked bottle; 4.Thermometer; 5. Constant pressure funnel; 6. Condenser; 7. Filtering flask; 8. Buffer flask; 9. Filtering flask; 10. Drying tube; 11. Vacuum tubing; 12. Three-way connector; 13. Oil pump; 14.

Vacuum Gauge; 15. Nitrogen regulator; 16. Nitrogen cylinder; 17. Methyl nitrite regulator; 18.Methyl nitrite cylinder.

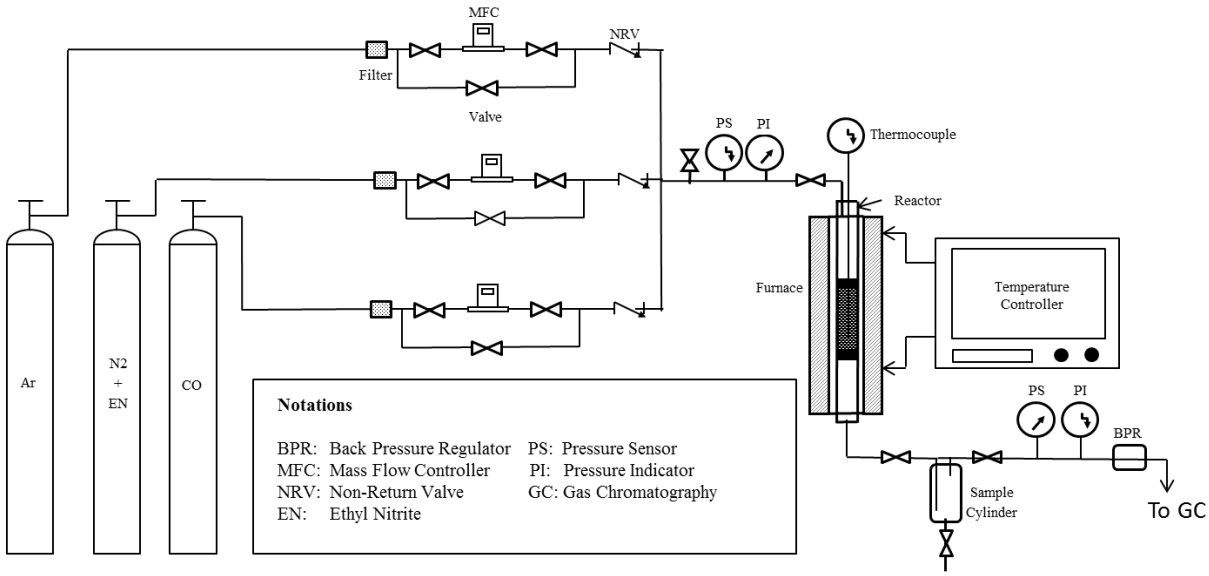

Figure 2.8.2. Schematic diagram of the EN to DEO installation.

Results and Discussion

The experimental set-up used for synthesis of DEO from EN was built and its schematic drawing is shown in Figure 2.8.2. Figure 2.8.3 shows the photos of the DEO hydrogenation installation. The system photographed as shown in Figure 3 has five main gas lines (N_2 + EN, CO and Ar) with another two lines which can be used for other gasses. CO and N_2 + EN cylinders (US Welding) were connected with two mass flow controllers (Porter Instruments) separately with stainless tubing (Swagelok). High pressure valves (Swagelok) were used before and after the mass flow controllers to protect them. Before the gases came into the reactor, check valves (Swagelok) were used to make sure no gas could go reversely into the mass flow controller. The mixture gas went into the reactor through stainless tubing (Swagelok) while a thermal couple was inserted into the reactor to control the temperature. A cold trap (Swagelok) was connected after the reactor to collect the product while all the tubing between reactor and cold trap was wrapped with heating taps. GC (SRI) was connected with the cold trap and a back pressure regulator (Swagelok) was used between them to adjust the temperature. All the exhausts came out from the GC will be released into the hood via stainless tubing. The reaction system is controlled by a National Instruments DAQ system and all the reaction parameters are recorded automatically. Security measures will be implemented for 24/7 unattended operation.

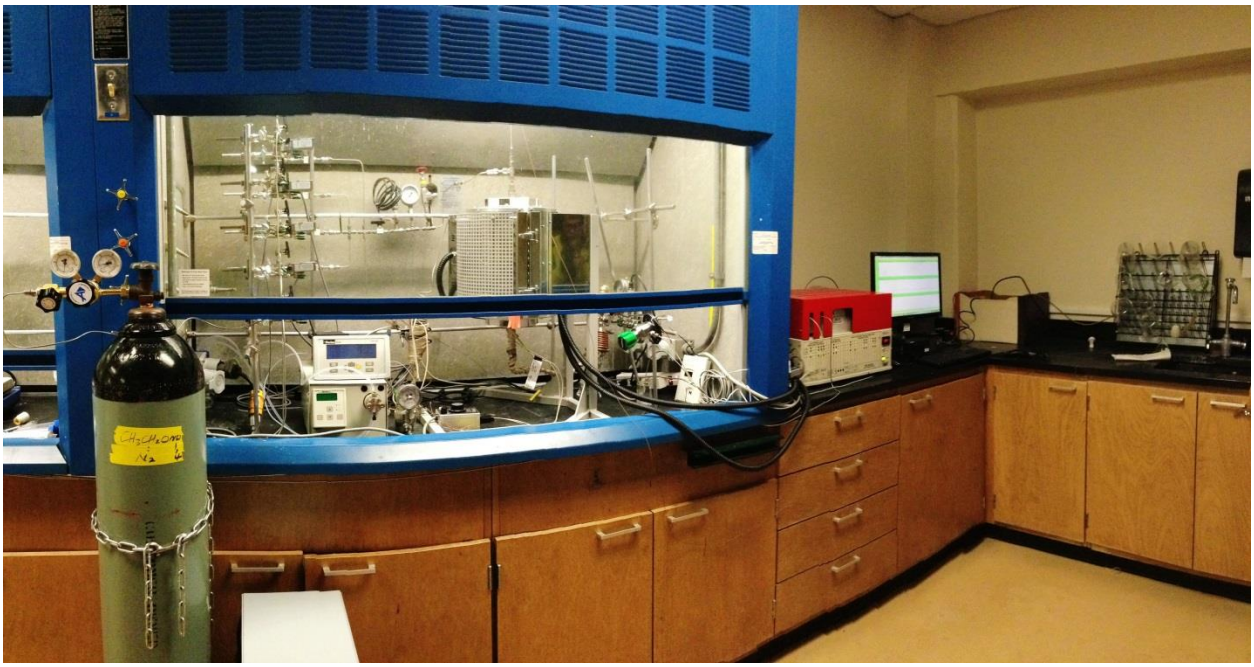

Figure 2.8.3. Photos of the DEO hydrogenation installation.

Plans for Upcoming Quarter

No input.

Theme 3 – Pre-Combustion CO_2 Capture

Subtask 3.1. – IGCC with CCS

Approach

Combining advanced gasification with CCS in the power sector remains a critical pathway towards low-carbon power generation. Industrial, research, and academic leaders from both countries will work with the major demonstrative projects and best in class technologies to provide the world with robust, transparent cost and performance estimates for the class of power plant. Pilot testing platform wil be constructed via this research work, based on which the technology of CO2 capture, utilization and storage based on IGCC will be developed and demonstrated.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Subtask 3.2. – IGCC Knowledge Transfer

Approach

Duke Energy and Huaneng are working to share start-up and operational lessons learned from Huaneng's GreenGen facility and Duke Energy's Edwardsport IGCC facilities. In addition, they will work with each other to expand knowledge and identify best practices.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Theme 4 – Post-Combustion CO_2 Capture, Utilization and Storage Technology

Subtask 4.1. – 1 MTons/Year Post Combustion CO_2 Capture at Duke Gibson Station

Approach

The activity of this task will be to perform a Pre-engineering Study of the 1 Million Tons/year Post-combustion CO_2 Capture systems, combined with a preliminary Techno-Economic Analysis and Budgetary Cost Estimate (±30%). Upon completion of these itms, a Sensitivity Study of Power Generation with Post-Combustion Carbon Capture System will be performed.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 4.2. – Development of Solvent for CO_2 Separation from Utility Flue Gas

Approach

The project is set up to develop innovative solvent compositions to reduce the overall cost of CCS. The first step in the process it the establishment of a technical team and a performance matrix for solvent formulation and evaluation. The next step will be the formulation of the solvent. Finally, evaluation will occur at various levels of scale to determine the solvent's performance capabilities. In this quarter a joint working group was established and met to determine the performance matrix which is reported below.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 4.3. – Development of Catalyst to Enhance CO_2 Capture Kinetics In Scrubber

Approach

Previous works on the second generation catalyst containing ionic ligands were showed to obtain high CO_2 hydration activity. Using a salen analog containing an imidazolium or phosphonium salt functionality were found to increase the rate enhancement of CO_2 hydration by two orders (~10^5) in comparison to earlier reported Zinc(cyclen) systems using CAER pH-drop assay. The success of the salen analog discussed in the previous quarter will guide the design of future catalysts for CO_2 hydration. It was discovered that by using slight variation in the salen framework we can tune the activity of the catalysts to fit specific needs.

Results and Discussion

Screening the activity of the catalyst, C8z by pH-drop method:

A stream of 14% CO_2/N_2 span gas was bubbled through a solution of 3.5 mM (2.3g/L) of C8z in 30% MEA and the drop in pH was recorded. In the absence of catalyst the MEA blank, solution takes about 35 minutes to drop the pH from 11 to 9.0 whereas in the presence of catalyst C8z it takes ~30 minutes (Figure 4.3.1). The results suggest that the catalyst is active for enhancement of CO_2 hydration rate, but only minimally and at higher carbon loadings. This correlates to very rich loadings of ~α = 0.48 – 0.51, and is out of the working range in an industrial process.

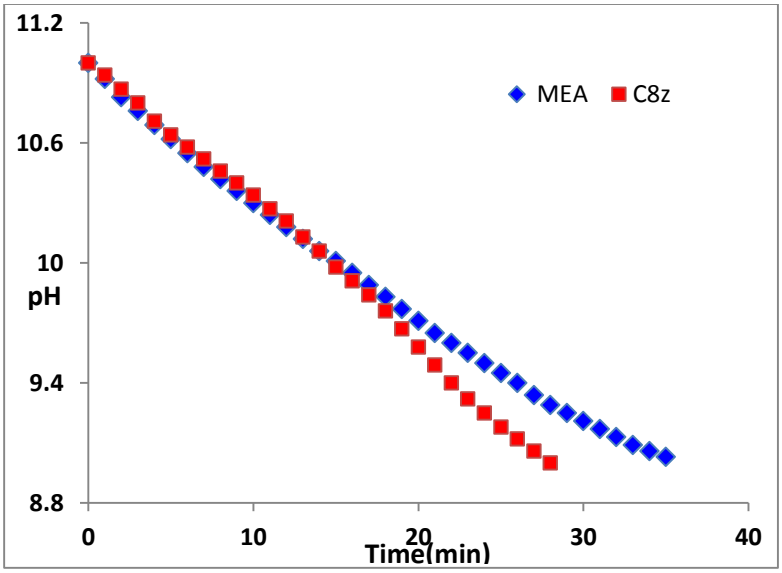

Figure 4.3.1: pH-drop of 30% MEA (blue diamonds) and 30% MEA with catalyst C8z (red squares) at 22 °C.

The results show that 4-coordinate ligands are not absolutely required for activity and stability in concentrated amines. It was previously believed that the in order to be stable in concentrated amine solutions a 4-coordinate ligand was needed, such as cyclen or salen. It was hypothesized that the multidentate nature of the ligand stabilized the metal center and prohibited in from reacting with the amines and other impurities. However, our recent results on 2- and 3-coordinate ligands show that an entirely new scaffold is suitable for CO_2 hydration catalyst development.

Screening the activity of the catalyst, C5c by pH-drop method

The activity of catalyst C5c was tested by pH-drop method. A stream of 14% CO_2/N_2 span gas was bubbled through a solution of 4.0 mM (2.3g/L) of C5c in 5M MEA (30%) and the drop in pH was recorded. In the absence of catalyst the MEA blank, solution takes about 27 minutes to drop the pH from 10.7 to 9.0 whereas in the presence of catalyst C5c it takes ~20 minutes (Figure 4.3.2). The results suggest that the catalyst is active for enhancement of CO_2 hydration rate within the working range of the solvent, especially at rich loadings.

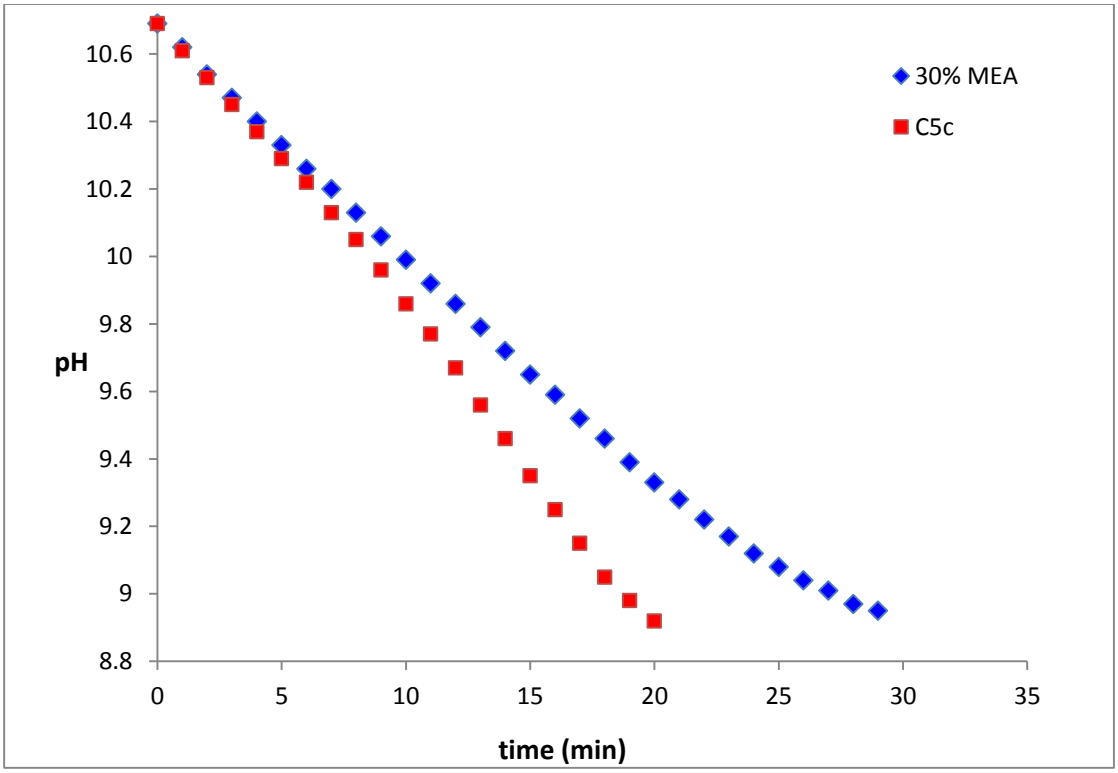

Figure 4.3.2: pH-drop of 30% MEA (blue diamonds) and 30% MEA with catalyst C5c (red squares) at 22 °C.

Thermal stability of catalyst C7z in 30% MEA:

Previous catalyst generations were found to be thermally unstable. The cause of this frailty of the zinc-based catalyst most likely arose from the unfavorable geometry of the complexes. This geometry is also what most likely gives the higher activity, but is also the cause for its deactivation. These catalysts were rigid and not unable to be dynamic and flex to more favorable geometries during the catalytic process arising to eventual catalyst deactivation. Catalyst CAER-C7z was designed to give a more flexible complex while allowing for the higher activity of zinc-based catalysts.

CAER-C7z, was tested to check its thermal stability by heating at 145 °C. A stock solution of C7z (1.8g/L) was prepared in a 30% MEA solution. A 50 ml solution of C7z was taken out from the stock solution and carbon loaded until the pH reached 10.5. The solution was transferred into an autoclave. Similarly another solution of 30% MEA is taken and carbon loaded in the same manner. This solution was also transferred into an autoclave. Both the solutions were heated under identical conditions. After a finite period of of heating, the solution was taken out of the autoclave and cooled down to room temperature, at which point a 25 mL aliquot of the solutions were taken from both the catalyst and blank solutions and pH-drop studies were carried out at 22 °C. It was observed that the activity of the catalyst was retained even after heating at 145 °C for up to 92 hours (Figure 4.3.3).

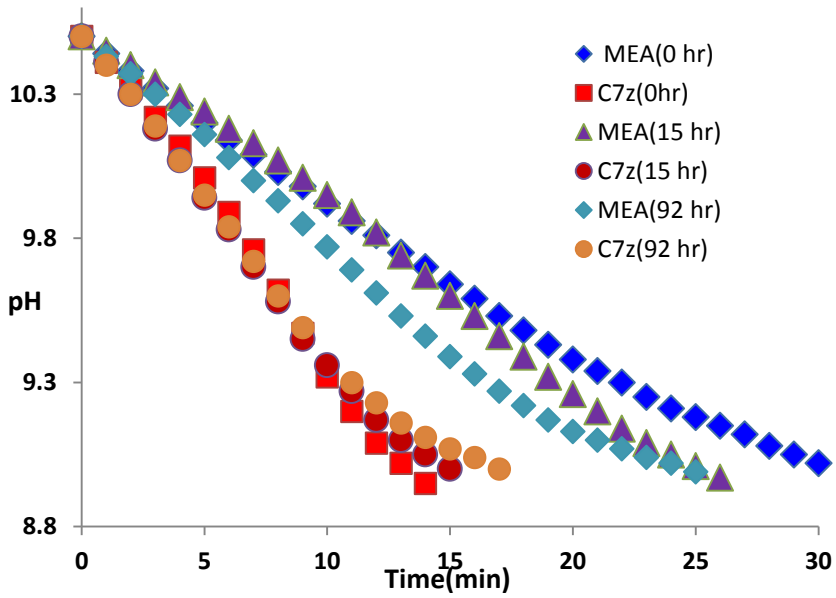

Figure 4.3.3: pH-drop of C7z in 30% MEA at 22 °C before and after heating at 145 °C.

All the results suggested that catalyst, C7z is an improved zinc-catalyst than earlier reported catalysts at CAER. In case of earlier reported catalysts at CAER, the ligands have four co-ordination sites to the zinc metal. The stability of C7z catalyst could be due to the flexible bidentatecoordination of the ligand frameworks which would allow for zinc to have tetrahedral and triginal bipyramidal geometry throughout the reaction progress; these are more stable geometries for zinc centers.

Plans for Upcoming Quarter

Work in the following quarter will focus on the development of a large scale synthetic method for catalyst C5c and C7z, and the activity of these catalysts will be measured via WWC.

Subtask 4.4. – Membrane Development for CO2 Separation from Utility Flue Gas Stream

Results and Discussion

RTIL-Based Hybrid Membrane Materials – Outcomes & Forward Look

ILs are promising materials for CO_2 capture due to their low regeneration energies, low volatilities, and high CO_2 selectivities and capacities. However, their industrial implementation as solvents for CO_2 capture is hampered by their high viscosities which lead to high pumping costs, slow sorption kinetics, and inefficient heat transfer. The ultimate focus of this Theme 4.4 tasking has been to develop novel deployment platforms for ILs to address the challenges associated with their large scale industrial use. To-date this work has explored development of novel IL-based materials using design strategies employing IL gelation, polymerizable ILs, and IL impregnation into polymer matrices to achieve enhanced CO_2 separation performance. Specifically, physically gelled ILs, polymerizable IL/IL composites, and polymer/IL composites were synthesized and evaluated as potential routes to advanced CO_2 capture materials. The effects of IL cation and anion functionality and polymer matrix chemistry were extensively explored and their impact on the material properties and CO_2 separation performance assessed. The main outcomes of this work are summarized below and near term paths forward addressed.

Polymer/IL Composites: IL impregnation into polymer matrices was applied to successfully fabricate IL/polymer hybrid materials for CO_2 separation. Both polyethylene glycol (PEG) and

polyvinylideneflouride (p(VDF-HFP)) based IL/polymer hybrid materials were synthesized. These polymer/IL hybrids showed promising high CO_2 affinity for potential deployment as sorbents and membranes for CO_2 capture from flue gas capture. IL/PEG sorbents were evaluated for CO_2 sorption near ambient temperature and realistic flue gas pressure conditions to understand the influences of IL cation and anion functionality and cation alkyl chain length on material performance. Sorption characteristics are an important component of membrane permeability, with the overall CO_2 permeability comprising both diffusive and sorptive based transport components. IL/PEG sorbents show high affinity for CO_2 and improved sorption rates over the neat ILs. High CO_2 sorption capacity up to 1.5 mmol/g sorbent was measured for IL/polymer sorbent containing [emim][Ac], which is comparable to other high performing porous organic sorbents but significantly lower than that reported for high performing inorganic sorbents. The high sorption capacity of [emim][Ac]/PEG materials is attributed to the chemical reaction between CO_2 and acetate group leading to carboxylate formation. Retention of a high sorptive component to CO_2 permeality especially at slightly elevated temperatures will be a critical factor in selectivity retention at anticipated process conditions.

IL/p(VDF-HFP) materials were evaluated as thin films to understand the influence of IL impregnation on the gas transport properties. Both amorphous and semi-crystalline p(VDF-HFP) were used as polymer matrices. A 2 to 3 order of magnitude increase in CO_2 transport was observed following IL impregnation into each polymer matrix. A CO_2 permeability of 1000 barrer and CO_2/N_2 selectivity of 12 was obtained for [emim][Tf2N]/p(VDF-HFP) containing 60 % [emim][Tf2N] at 75 °C. During temperature cycling between 75 °C and near ambient temperatures, the amorphous polymer matrices showed dramatically improved IL retention capability as compared to the semi-crystalline polymer matrices comprising the same chemical compositions. Further development and deployment of these IL/polymer composites as membranes with thin selective layers (ca. 100 nm) would lead to unprecedented CO_2 permeances (10,000 GPU). Since CO_2 capture cost using membranes is significantly affected by the permeance (inverse relation), significant reductions in CO_2 capture cost are achievable with membranes having high CO_2 permeance. To fully realize the techno-economic benefits of the improved permeance, further improvement in CO_2/N_2 selectivity is required. While process schemes are accessible to utilize membranes with selectivities below 20, process designs combined with systems analysis efforts from non-profits, government, and industrial entities show efficiency and cost advantages if selectivities reach 20.

Gelled ILs: Gelled-IL materials were fabricated using physical gelation of ILs with a low molecular weight gelator. Extensive rheological characterization of the gelled-IL materials was conducted to understand and improve mechanical properties of the gelled-IL materials. The gelled-IL thermal history and fabrication protocols had profound impacts on gelled-IL mechanical properties. Gels prepared by mixing gelator and IL at temperatures above their gel point, typically 155 °C, followed by quenching in ice bath were found to have the highest moduli, followed by gels that had been rapidly quenched from 145 to 0 °C at -30 °C/min cooling rate in the rheometer. Gels prepared by slow cooling of a sol to 0 °C exhibited the lowest moduli, indicating that they are the weakest mechanically. Thus, rapid cooling appears to result in the formation of a stronger gel network with the low temperature and rate of the quench influences the extent of that enhancement. Increasing gelator concentration also led to improved gel strength and an increase in sol-gel transition temperature, an important factor for determining their utility in elevated temperature process environments. The sol-gel transition temperature identified for the gel containing 40 mg gelator is approximately 125°C, which is significantly higher than that measured for gelled-IL with 15 mg/g gelator. Although the synthesized gelled-ILs have solid-like characteristics, the mechanical properties of the gelled-ILs are not yet

sufficient to allow their deployment and use as solid sorbents or membranes utilizing any fabrication scheme. Further improvements in the gelled-IL mechanical properties are mandated to realize their potential as a medium for carbon capture. A new gelation chemistry with promise in addressing this issue has been identified this quarter and will be evaluated as a membrane additive in the coming quarters.

Polymerizable IL/IL Composites: IL polymerization into solid films was accomplished by incorporation of polymerizable functional groups including vinyls, methacrylates, acrylates, and epoxides into monomeric and oligomeric backbones incorporating IL moieties. Post-polymerization, these poly-IL materials were shown to have exceptional IL retention ability with free IL loadings up to 80%. As a result, these poly-IL/IL composites are attractive materials for CO_2 capture. Ultrasonic assisted atomization was used to synthesize poly-IL/IL materials. The influence of initiator type, concentration and reactive functional group were evaluated to obtain robust poly-IL films. Although, the poly-IL materials fabricated showed solid-like characteristics and the ability to retain high fractions of free-IL, the long reaction times for the vinyl and methacrylate functionalized materials and short shelf-life of the highly reactive acrylates and epoxides rendered poly-IL membrane fabrication using LANL USCT a significant challenge. Other techniques such emulsion polymerization should be explored to fabricate thin poly-IL selective layers while potentially mitigating the fabrication challenges encountered due to polymerization kinetic constraints.

Plans for Upcoming Quarters

The work conducted as part of this ongoing effort comprises the feasibility research required to progress the technology to the next stage of development and validation. As a result of the work in this subtask area to-date and the overarching conclusions and assessment of near term success potential of the technology/materials design approaches pursued as part of this tasking, a single approach has been down-selected for continued development. Commercialization/Success potential was evaluated with input from potential end users of the technology both interested in deployment for their industrial CO_2/N_2 and CO_2/CH_4 separation needs. The selected materials design strategy employs polymer/IL composites comprised of low crystallinity polymer matrices resulting in high IL loading potential, excellent IL retention under anticipated process conditions, high CO_2 affinity, and industrially attractive permselectivity. The near term path forward for continued progression of these materials as a separation media will be conducted as part of our ongoing efforts to develop commercially attractive materials and methods to realize commercially viable deployment of the developed materials as membranes. It is our assessment that advancing these materials to the next stage of development and demonstration as high performing CO_2 capture membranes will involve the following critical tasking:

- Given the industrially attractive separation performance (permeability and selectivity) exhibited by these materials at ambient conditions, the next progression should involve translation of these materials into high permeance/ throughput membranes. This translation will comprise further developing methods to fabricate ultra-thin selective layers of these materials on commercially attractive supports.
- Demonstration of the composite material and membrane performance over a broad range of industrially relevant operating conditions and environments to define optimum separation process parameters for use of this technology in coal derived flue gas (temperature, trans-membrane pressure, impurity and water tolerance and performance influences).

- Continued materials optimization to further improve material selectivity at elevated process temperatures leading to improved process economics. Near-term efforts should be scoped to involve incorporation of hybrid additives targeting elevated selectivity.

Subtask 4.5. – Post CO_2 Scrubber Solvent Enrichment

Approach

Capacitive deionization (CDI), described in previous reports, is being utilized here in an effort to decrease the amount of carbon-rich MEA solution (mainly water) that needs to be processed during the solvent regeneration step. To accomplish this, carbon-rich MEA ions will be concentrated using the CDI process with porous carbon materials. This work aims to examine specifically carbon xerogel-type (CX) electrode materials. Factors such as pore size, porosity, surface area, wettability and conductivity are all important for ion capture among others such as electrochemical properties.

This past quarter has been spent further examining an alternative solvent to MEA, piperazine, due to its thermal stability in solution at elevated temperature. Longer-term testing was carried out with a flow-through CDI cell using this carbon-loaded piperazine solvent. Similar degradation to previous results with NaCl was seen. Mitigation strategies to increase the separation lifetime of the device was investigated. For the first time, a CDI process has been shown to maintain successful separation of salt for >400 cycles.

Experimental

SiO_2 was deposited on the carbon xerogel surface through TEOS treatments. The modification procedure includes (1) TEOS (Sigma-Aldrich, >99%), ethanol, and HNO_3 were mixed at a volume ratio of 1:20:1, and the mixture was stirred vigorously for 1 h, (2) the CX sheets were dipped into the mixture for 3 min, and dried in an oven at 100 °C for 30 min, and (3) the samples were further heated at 300 °C in the oven for another 12 h. It should be mentioned that procedure (2) was repeated for several times (X = 1, 5, and 10) to increase the amount of SiO_2 loading on the carbon xerogel surface, and the resulting samples were denoted CX-SiO_2-X in the text and figures. As-deposited silica-coated carbon xerogel electrodes were then examined by BET/BJH N_2 adsorption isotherm analysis, SEM/EDS, FTIR, and electrochemical methods.

CDI tests were performed in a flow-through cell assembled with the CX electrodes adjacent to titanium current collectors. The electrodes were separated by a 1.5 mm thick silicon rubber. Adsorption-desorption cycles were performed at 1.2 V and the short-circuit potential, respectively, for a total of 15 combined cycles. The CX electrodes had a total mass of ~0.8 g (~42 cm^2). During system operation, 500 ml of ~4 mM NaCl solution was continuously purged with wetted N_2 in the solution reservoir, and circulated using a peristaltic pump (Masterflex) at 27.2 mL min^{-1}. A conductivity meter (Cole-Parmer 19500-45) at the cell outlet was installed to calculate the electrosorption capacity (Γ).

$$\Gamma = (\Delta\sigma M_w V)/(mc) \qquad (1)$$

where $\Delta\sigma$ is the conductivity difference between the adsorption-desorption steps at steady state (last 100 s), M_w is the molar mass of NaCl, V is the volume of the salt solution, m is the mass of the carbon used, and c equals 112.77 determined from the slope of conductivity as a function of NaCl concentration. The current efficiency and charge efficiency were calculated using equations 2 and 3, repectively

$$\text{Current Efficiency} = \frac{\text{Charge}_{\text{Desorption}}}{\text{Charge}_{\text{Adsorption}}} \quad (2)$$

$$\Lambda = (\Gamma F / M_w)/(Q_{ad}) \times 100 \quad (3)$$

where Λ is the charge efficiency, Γ is the electrosorption capacity, F is Faraday's constant, MW is the molecular weight, and Q_{ad} is the charge used during adsorption.

Results and Discussion

Carbon Loaded Piperazine Enrichment: Cycling Stability

In the past quarter, enrichment of carbon loaded piperazine has been reviewed in more detail and calculations from the previous quarter updated. In addition, a larger-scale cell (5 pairs of electrodes, flow-through cell) has been used to gain more piperazine enrichment information along with corresponding LC/MS analysis. Shown in Figure 4.5.1 is the separation and enrichment of carbon loaded piperazine using this flow-through CDI cell. LC/MS analysis confirms the enrichment of piperazine using this process, corroborating data reported in prior quarterly reports.

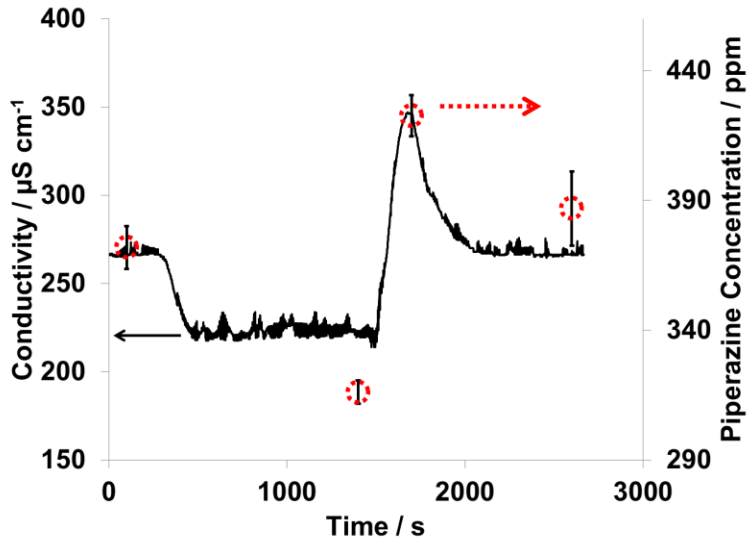

Figure 4.5.1. Adsorption-desorption conductivity curve of PZ solution (black solid line) using an applied potential of 1.2 V and 3.2 g of carbon xerogel. Corresponding PZ concentrations are shown with red dashed circles as measured by LC/MS.

In general, quantified LC/MS data correlates well with our conductivity plots showing both a decrease in PZ concentration under potential and an enriched concentration with the release of the applied potential. In this case, the enrichment peak is approximately 13% higher in PZ concentration over the standard solution value. While this 13% may not sound sizable, it is statistically significant here and confirms the ability of CDI devices to enrichment a variety of salt streams. In order to increase the enriched concentration, multiple routes can be taken. One possible route would be decreasing the internal volume of the separation cell. That is currently being examined and represents the most reasonable route. Other options include increasing the salt capacity of our carbon material or using higher potentials. We have worked for a while to increase the capacity of our carbon with some decent results as mentioned with silica coatings and sulfanilic acid, but decreasing the internal volume of the cell would present the most dramatic increase in the shortest period of time and will be used in further scale-up operations.

Overall View for Long-Term Cycling of a CDI Cell

Figure 4.5.2 gives the overall view of the electrosorption capacity (Γ) versus cycles (#) for long-term CDI operation in ~4 mM deaerated NaCl. It can be seen that degradation is observed along with the cycles similar to results reported in the previous quarter. This degradation mechanism has been discussed in detail in previous reports, i.e., the oxidized anode leads to the potential of zero (PZC) of the anode being positively shifted across the short-circuit potential (E_o). In the current study, it is found that the decrease in the Γ value depends on not only the applied potentials but also the electrode's connections at the adsorption step. For instance, at 1.2 V, the starting Γ value is ~3 mg g^{-1} in Region A. In contrast, at 1.2 V but reversed connection, the starting Γ value is ~5 mg g^{-1} in Region D. Based upon this observation, it can be understood that the selection of the suitable operation condition can also enhance the electrosorption performance for a CDI cell. We will discuss briefly the reasons behind Γ values and cycle number for each region shown in Figure 4.5.2.

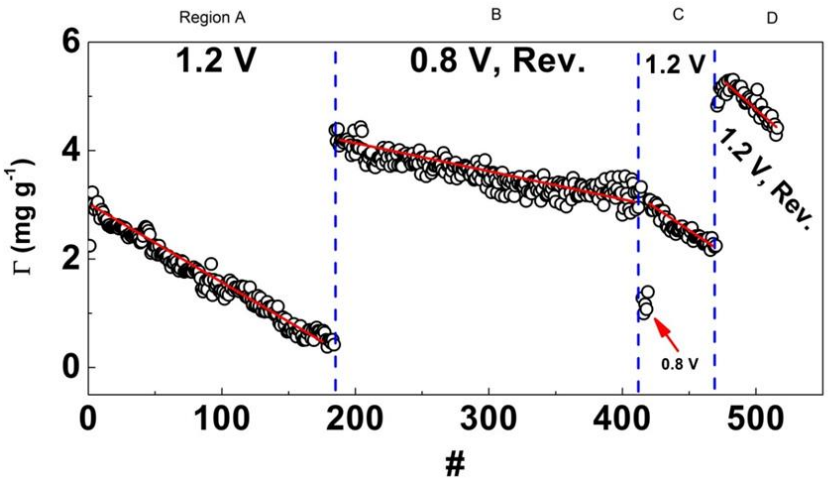

Figure 4.5.2. Long-term cycling performance – electrosorption capacity (Γ) versus cycles (#). The quantification of the Γ values can be found in our recent publication in Electrochemistry Communications. This experiment was performed at either 1.2 or 0.8 V for the adsorption step, and at short-circuit potential for the desorption step in ~4 mM deaerated NaCl solution. In this plot, Rev. means that the connection of the CX electrodes was reversed.

In Region A, as the CDI cell is charged at 1.2 V and discharged at the short circuit potential, the electrosorption capacity of the electrodes decreases as a function of cycle number due to the appearance of oxide surface groups at the anode which has been reviewed in detail in the previous quarters. In Region B, the electrode connections are switched where the anode is now acting as the cathode and vice versa. The shifted PZC from the prior anode increases the driving force at the cathode for cation adsorption while the prior cathode (nearly pristine carbon xerogel) functions well as an anode. The increase in performance shown in Region B tracks well with the changes in PZC at the carbon xerogel surface for both the anode and cathode. Performance degradation is again seen, at a lower rate, due to the lower applied potential. As the oxide groups build up, the PZC again shifts at the anode, and performance loss is seen. In Region C, the potential is increased to 1.2 V which only increases the rate of performance loss. In Region D, the electrodes are again reversed, and the capacity increases. It appears that switching of the anode and cathode may be able to increase, or at least maintain, the separation ability of this CDI process. This stabilization of performance is shown for CDI for the first time here and results in the possibility of CDI separation devices having exceptionally long cycle lives. Possibilities for increased device lifetime will be examined in great detail in the next quarter.

Printed Circuit Board of Novel dc-dc Converter

An initial dc-dc converter for charge/energy recovery from a CDI cell has been completed and a circuit board of the initial design has been printed. Shown in Figure 11 are the design and initial printed circuit board (PCB). This PCB was used to actively control CDI cells in our lab demonstrating initial successful operation. With first use, energy recovery was minimal due to the discharge characteristics being used in the control program as well as a switch in the PCB that would not stay fully closed or open. A new iteration of this PCB has already begun construction and will be implemented early in the next quarter.

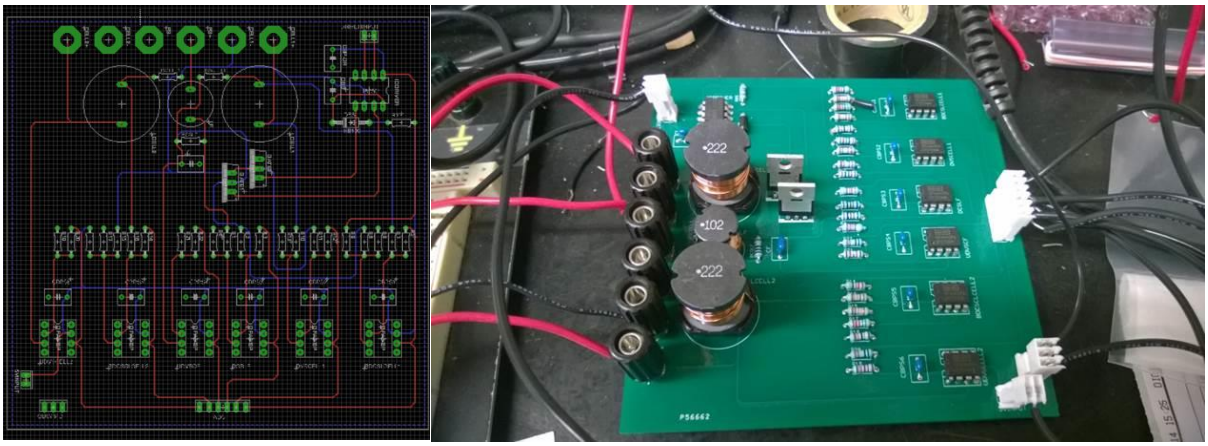

Figure 4.5.3. Printed circuit board (PCB) design on left and the finalized PCB shown on the right. A microcontroller and computer were used with this PCB to actively control CDI cells in our lab.

Plans for Upcoming Quarter

The next quarter will focus in detail on increased separation lifetime of the CDI cell using active switching and integrated relay components. In addition, the incorporation of the dc-dc converter described briefly here will be further examined in our system to determine levels of energy recovery that are possible from these systems. Finally, larger-scale CDI separation experiments will start to take place as carbon production is increased by using GrafTech to carbonization our xerogel. Their experience and facilities will aid in carbon production for this process.

Theme 5 – Oxy-Combustion Research, Development, and Demonstration of Oxy-Firing Combustion

The goals for theme 5 activities are defined as following:

- Accelerate the development and testing of oxy-coal combustion technologies suitable for Chinese coals.
- Establish a working relationship between the leading oxy-coal combustion development institutes in US and China

Subtask 5.1. – Fuel Characterization and Emissions Study Under Oxyfuel Conditions

Approach

The proposed bilateral joint project will study the fundamental and pilot-scale combustion and emission characteristics of indigenous Chinese and US coals of different ranks under oxyfuel conditions.

- Identify Chinese and US coals, one of each, for benchmark comparison of test data.
- Evaluate and exchange test data, including fuel analysis, devolatilization and char oxidation test results from the bench-scale facilities at both HUST and B&W.
- Validate reaction sub-models in the CFD codes (HUST's FURN and B&W's COMO) using the aforementioned experimental data. The model parameters will be reviewed and revised when necessary.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Subtask 5.2. – Pilot-Scale Oxyfuel Combustion Evaluation and Optimization

Approach

Work will create a model for burner design for oxy-combustion conditions, pilot-scale oxy-combustion evaluation and optimization.

- Evaluate designs of B&W's SBS and HUST's FCS. Exchange furnace and setup CFD models for each facility.
- Define a reference burner for both furnace geometries and perform CFD simulations. Compare the simulation results (flame quality, flow patterns, temperature profiles, heat transfer, emissions, etc.) to identify model deficiencies for improvements. Comparison to existing SBS test data will be made when available.
- In the long-term, develop new burner design and test it using indigenous coals for oxy-combustion applications.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Subtask 5.3. – Steady-State and Dynamic Process Modeling Simulations

Approach

Work will setup steady-state and dynamic process models using Aspen and analyze simulation results for the pilot-scale FCS and SBS.

- Set up Aspen steady-state and dynamic simulation models for both facilities on each side.
- Compare the modeling results to identify oxy-specific process modeling issues and resolve any discrepancies.
- Perform preliminary model validation with existing data from previous SBS oxy-combustion test programs.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Subtask 5.4. – Feasibility Study for Large Scale Deployment

Approach

Conduct a commercial-scale engineering feasibility study for an oxyfuel –combustion reference plant.

- Conduct the technical and economic feasibility study of 1 million tons / year CO_2 capture system
- Obtain the capabilities of optimization and engineering design for post-combustion CO_2 capture system.

Results and Discussion

Task is complete at this time.

Plans for Upcoming Quarter

Task is complete at this time.

Subtask 5.5 Evaluate novel staged oxy-combustion concept:

Approach

In this new subtask, the project team will evaluate novel staged oxy-combustion concept by

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

Results and Discussion

One major project objective is to study pulverized coal combustion in atmospheres of high oxygen concentration (above 50% O_2), in order to simulate conditions in the early stages of the staged combustion process. Results of experiments, which were obtained with an oxygen concentration of up to 50% in the secondary oxidizer stream, were previously reported. As predicted, the volatile flame length was found to be inversely related to oxygen concentration, and at 50% O_2 the resulting flame was shorter than desired. It was determined that modifications

to the burner were needed before increasing the oxygen concentration further. In order to increase the flame length and avoid high-temperature flame impingement on the furnace walls, we attempted to drastically reduce the swirling flow in the burner and achieve an axial flow. This caused the flame to become detached from the burner, and a lifted flame resulted.

In order to improve the flame stability in the axial (low swirl) mode of burner operation, the burner was modified to include a port for injection of pure O_2. The modified burner was successfully tested utilizing natural gas, and the effects of oxygen injection on flame stability and shape were observed.

In a parallel effort, experiments were conducted at the University of Stuttgart by a visiting Washington University Saint Louis (WUSTL) graduate student. These experiments aim to provide insight into the effects of excess oxygen on the properties of fly ash and ash deposits. Combustion experiments were performed in a ~100kW down-fired, electrically heated faciltiy. Preliminary results are currently being assessed.

Plans for Upcoming Quarter

The modified burner will be operated with the injection of O_2 and a small amount of natural gas, to create a high-temperature pilot flame during future tests with coal. This pilot will act to stabilize the pulverized coal flame under conditions of axial flow. This will result in a longer flame that is well-suited for measurements of heat flux, temperaturature, and gas composition, under highly oxygen-enriched conditions.

Theme 6 – Sequestration capacity and near-term opportunities

Subtask 6.1. – Saline Formations at the Basin Scale

Approach

The goal of subtask 6.1 is to build the scientific, technological, and engineering framework necessary for safe, permanent storage of large quantities of anthropogenic CO_2 in the sedimentary basins of the Shaanxi Province and the state of Wyoming through 1) determining the distribution of potential sealing formations and appropriate geological structure; 2) assessing the potential storage capacity of major saline aquifers in the Ordos Basin and Wyoming Laramide Basins; 3) constructing a 3-D geological model of the storage domain for selected storage sites; and 4) completing performance assessments for a variety of injection/storage scenarios at targeted sites using numerical simulations.

Working closely with colleagues at the Shaanxi Provincial Institute of Energy Resources and Chemical Engineering (SPIERCE), Northwest University (NWU), Yanchang Oil Company (YOC), and Institute of Rock and Soil Mechanics of Chinese Academy of Sciences (IRSM), the CERC-ACTC team at the University of Wyoming Carbon Management Institute (CMI) continues to collect and analyze the geologic, geophysical, geochemical, petrophysical, and petrographic data available for the Ordos Basin and Wyoming Laramide Basins.

Results and Discussion

At present, research scientists from CMI, SPIERCE, and NWU are working on the following assignments: 1) reprocess and analyze data regarding the regional geology, structural/stratigraphic framework, and thermal/burial history of the Ordos; 2) update the inventory for the distribution of energy resources in the Ordos Basin, including oil, gas, coal and other natural resources; 3) delineate potential CO_2 sources and sinks in the Ordos Basin; and 4) refine the regional 3-D geological model for the Ordos Basin. These tasks were carefully outlined in joint meetings with CMI/CERC partners. CMI and its Chinese partners believe accomplishing these four tasks will expedite the establishment of an effective pathway to a better understanding of CCS for both nations.

In this quarter, the research team has made progress in accomplishing the objectives of each of the above tasks. The structural contour maps for the major stratigraphic horizons have been reconstructed and a 3-D geological structural model is refined. Results suggest that the Yanchang Formation, the Liujiagou Formation, and the Majiagou Limestone are the major potential CO_2 storage reservoirs in the Ordos Basin. The depositional environments, thermal/burial/diagenetic histories of the basin suggest that both of these stratigraphic units have substantial CO_2 storage potential, particularly in the structural unit “Shaanbei Slope” of the Ordos Basin. The reservoir heterogeneities are prominent both vertically and laterally for all targeted formations. Based on the experience from the WY-CUSP project, these serious reservoir heterogeneities will have a significant effect on the storage capacity assessment of the targeted storage formations in the Ordos Basin, China.

Highly productive discussions about information transfer and the design of cooperative projects carried by Wyoming, Shaanxi, and Wuhan CERC-ACTC members were ongoing this quarter. A major point of these discussions is to improve the understanding of both the Madison Limestone (analog to the Majiagou Limestone in the Ordos Basin), and the Weber Sandstone and Mesaverde Group (analog to the sandstone of the Liujiagou and Yanchang formations). It is apparent that the Lance Formation and Madison Limestone in Wyoming serve as instructive

analogs to the Yanchang Formation and Majiagou Limestone in the Ordos Basin. Both CMI and its Chinese partners are enthusiastic about sharing their expertise and experience in characterizing the CCS attributes of the most promising CO_2 storage sites in Wyoming and Shaanxi.

Plans for Upcoming Quarter

1) Update inventory results of the distribution of major stationary anthropogenic CO_2 emission sources, including the volumes of captured/vented CO_2
2) Refine 3-D geological/structural model of the Ordos Basin using the newly available stratigraphic data, and compare this model with similar models of the Greater Green River and Powder River basins of Wyoming.
3) Determine the trend of karstification in the Majiagou Limestone, a most critical parameter that affects the geological CO_2 storage capacity assessment of the Ordos Basin.
4) Assemble the reservoir property data for the targeted geological CO_2 storage reservoirs in the Ordos Basin
5) Select the storage site for a detailed geological structure and property modeling.
6) Attend the Theme 6 Wuhan workshop in May at Wuhan, and present lessons learned from the WY-CUSP RSU site characterization project.

<u>Subtask 6.2: Geologic storage and EOR</u>

Approach

The goal of Subtask 6.2 is to build the scientific, technological, and engineering framework necessary for CO_2 utilization via enhanced oil recovery (EOR) in conjunction with safe, permanent storage of large quantities of anthropogenic CO_2 in the Ordos Basin. The subtask goals will be achieved by accomplishing the following tasks:

- Evaluating the geological characteristics of potential CO_2-EOR reservoirs in the Shaanbei Slope, Ordos Basin;
- Comparing the Ordos reservoir characteristics of mutual oil fields with Wyoming CO_2-EOR fields;
- Constructing detailed 3-D geological models of the targeted oil fields;
- Numerically simulating CO_2-EOR performance for a variety of EOR scenarios at the selected depleted oil fields;
- Evaluating the feasibility of combining CO_2-EOR with CO_2 storage; and
- Planning a CO_2-EOR demonstration project for one selected reservoir in the Ordos Basin.

The University of Wyoming Carbon Management Institute (CMI) team will work closely with researchers from Shaanxi Provincial Institute of Energy Resources and Chemical Engineering (SPIERCE) and Yanchang Oil Company (YOC) to develop an integrated energy/environmental expansion strategy for the energy rich basins such as the Ordos Basin and Wyoming Laramide basins. This integrated energy/environmental expansion strategy will include co-exploration, development of oil, gas, and coal resources, petrochemical and coal chemical industry, water resource management, CO_2 emission control, CO_2 utilization, and geological CO_2 stage.

In this quarter, the University of Wyoming Carbon Management Institute (CMI) team has worked closely with researchers from the Shaanxi Provincial Institute of Energy Resources and Chemical Engineering (SPIERCE) and the Yanchang Oil Company (YOC) to evaluate the

geological, petrophysical, petrographic, and petroleum-engineering data available for the EOR/storage project.

Results and discussion

At present, the CMI team is assisting both the YOC and SPIERCE in screening and prioritizing fields in the Ordos Basin with respect to their potential for using CO_2-flooding techniques. The Wyoming CMI team, working with Chinese partners (YOC and SPIERCE) has developed an assessment strategy, including screening criteria for the Ordos Basin oil fields. CMI is assisting the YOC to select one depleted oil field for CO_2-EOR demonstration in the Ordos Basin. The fields under consideration typically are located less than 100 km from major anthropogenic sources of CO_2, such as the YOC's Jingbian methanol plant, that presently captures and vents 5 Mt of CO_2
(> 95% pure) annually (Figure 6.2.1). The CO_2 capture facility of 50,000 tonnes has been installed. A 340,000 tonnes capture facility is under construction now and will be completed in the fourth quarter of this year. The capture facility with the coal-to-chemical plant will secure the CO_2 source for the CO_2-EOR demonstration project in the Ordos Basin.

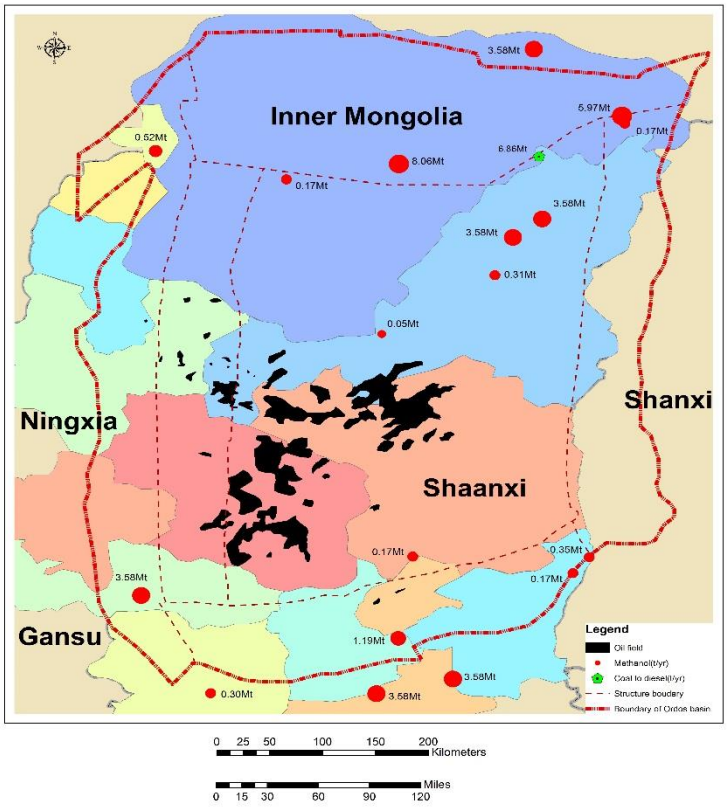

Figure 6.2.1. Map of the Ordos Basin showing geospatial districts, location of gas and oil accumulations, and location of stationary CO_2 emission sources. The total annual CO_2 emissions in the Ordos Basin are approximately 400 Mt.

CMI, YOC, and SPIERCE have agreed to share the information required to screen, characterize, model, design, and implement an enhanced oil recovery and CO_2 storage demonstration project

on the Shaanbei Slope in the Ordos Basin. CMI and the YOC have prepared a cooperative agreement to achieve Subtask 6.2 objectives. Work plans for years four and five of Subtask 6.2 have been finalized with CMI's Chinese partners and submitted to the CERC-ACT manager.

CMI, YOC, and SPIERCE are collaborating on the investigation of the geologic resources, energy resources, and CO_2 sources and sinks in the Ordos Basin. In addition, the research will explain how U.S. EOR experiences and expertise can be applied to depleted oil reservoirs in the Ordos Basin.

Plans for the upcoming quarter

In the upcoming quarter, scientists from SPIERCE—in cooperation with CMI—will continue to make improvements in the Ordos Basin database. The process and analyses of valuable sources of information regarding Ordos Basin geology, CO_2 availability, and enhanced hydrocarbon production will be continued. The petrographic observation of the targeted reservoirs (i.e., Yanchang Formation and Majiagou formation) will be conducted with the samples collected from the Ordos Basin. CMI personnel will visit SPIERCE, Northwest University, and Yanchang Oil Company in the summer of 2014 to continue the inventory, selection, characterization, and performance assessments for the targeted CO_2-EOR reservoirs.

University of Wyoming Carbon Management Institute (CMI) team will work closely with researchers from the Shaanxi Provincial Institute of Energy Resources and Chemical Engineering (SPIERCE) and the Yanchang Oil Company (YOC) to develop an integrated energy/environmental strategy for the energy rich basins such as the Ordos Basin and Wyoming Laramide basins. This integrated energy/environmental expansion strategy will including co-exploration/development of the oil, gas, coal resources, petrochemical and coal chemical industry, water resource management, CO_2 emission control, CO_2 utilization and geological CO_2 stage.

<u>Subtask 6.3. – Geological Storage and Enhanced Coal-Bed Methane (ECBM) Recovery</u>

Approach

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

<u>Subtask 6.4.a – Simulation and Modeling - LLNL</u>

Approach

Under the simulation task, advanced subsurface modeling tools and approaches are being applied to CO_2 storage projects in the U.S. and China and new simulation approaches and tools are being developed to address the issue of parameter uncertainty. Modeling tools are being used to assess a number of key performance questions as well as to provide quantitative insights that feed into risk characterization, including:

- Quantification of injection mass fluxes and pressures
- Mapping of potential fluid pressure and CO_2 saturation distributions throughout the target reservoir
- CO_2 storage capacity
- Evaluation of leakage pathways for injected CO_2

- Assessment of effective stress on nearby faults
- Gauging the induced seismicity potential
- Quantifying CCS efficacy when used in conjunction with enhanced oil recovery

U.S. and Chinese scientist involved in the subsurface simulation task met in Wuhan, China in March 2012 to develop a detailed work plan and schedule over deliverables over the next year of the project. These are summarized in a set of ten-point plans, to be submitted separately to DOE. In summary, the overarching goals of the simulation task are to develop templates and protocols for demonstration project evaluation, model development, and larger scale injection predictions; assemble a catalog of models and techniques and apply to site data sets, as warranted; compare results and summarize general findings; understand similarities and differences of CCS and CCUS risk assessment methods, needs, and goals between the U.S. and Chinese teams; identify key sites and specific hazards (including economic issues); develop abstractions of subsurface simulations to inform risk calculations; and calculate risk profiles for selected projects and use demonstration scale data to predict larger scale system behavior. These goals are to be addressed using sites in both the U.S. in China as example application, including:

- Ordos Basin, China: saline aquifer geologic storage in Paleozoic units
- Wyoming, USA: saline aquifer geologic storage in the Madison and/or Weber Formations
- Illinois Basin, USA: Saline aquifer geologic storage in the Wabash Valley in the Mount Simon Formation. Of particular interest to the simulation task is the planned injection of CO_2 at the Gibson-3 coal-fired power plant unit in Indiana, where a partnership between Duke Energy and China Huaneng Group to collaborate on CO_2 capture is in place. The simulation task will focus particular effort on this site, since clear synergies exist between the CO_2 capture and storage efforts (e.g., determining the optimal CO_2 flux for capture and subsequent storage) and the interests of the Chinese and U.S. partners directly converge.

Results and Discussion

No Results this Quarter

Plans for Upcoming Quarter

No Results this Quarter

<u>Subtask 6.4.b – Simulation and Modeling - LANL</u>

Approach

LANL is tasked with leading efforts into risk analysis for subsurface carbon storage. The risk component of the CERC work relies heavily on input from both characterization (original Project Task 1, new Themes 6.1) and simulation (original Project Task 2, new Theme 6.4). The original work plan for risk (Project Task 3) was written in a way that included multiple aspects of risk. Two primary risk components include subsurface risks for individual injection sites (Pawar et al., 2013) and risks associated with regional systems of multiple sources of CO_2 connected to multiple subsurface sinks (Keating et al., 2011a,b). Economic concerns were included in both components. Target sites for analysis of subsurface risk were chosen in each country including the Rock Springs Uplift (RSU) in Wyoming, the Ordos Basin in China, and the Gibson injection

site in southern Indiana. Although LANL is leading the risk effort, researchers at LLNL (Lawrence Livermore National Laboratory), UWY (University of Wyoming), and LANL are working together to produce the large number of related simulations needed to answer questions covering both subsurface and total storage system performance and risk for the chosen sites and their regions.

Subsurface Injection Site Performance and Risk

Methods for calculating CO_2 subsurface storage site performance and leakage risks are currently being developed by several teams around the world (Stauffer et al., 2009a; Oldenburg et al., 2009; Pawar et al., 2013; Stauffer et al., 2013). The state of the art in such modeling involves gathering detailed site specific data that are then used to create numerical models of plume injection and migration including time dependent pressure and saturation predictions. The plume estimates are next used to calculate potential leakage through wellbores, faults, and overlying caprock (Viswanathan et al., 2008). Finally, impacts are calculated on receptors such as drinking water aquifers or releases to the atmosphere that could change near surface concentrations of CO_2. A final step in a risk analysis is to assign consequence values to impacts so that a true risk value can be calculated as risk = probability*consequence. Currently all CERC work is focused on understanding the interplay between probabilities of events, how uncertainties in these events can be reduced through either data collection or engineering, and finally how costs relate to this interplay.

The reservoir simulations supporting the CERC risk work are being run using both the LANL developed porous flow software, FEHM (Zyvoloski 2007; Deng et al., 2012), and the LLNL developed simulator, NUFT. A second component of subsurface risk, seismic potential, is being explored using the same numerical meshes but with the fully coupled stress/flow capabilities of FEHM and through a hybrid stress code coupled to NUFT. Finally, economic considerations including costs associated with brine treatment (as part of a comprehensive reservoir pressure management scheme) are included as part of each individual storage site performance assessment (Sullivan et al. 2012a,b; Surdam et al., 2009; Surdam et al., 2011).

Regional Scale Source to Sink Performance and Risk

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 (Middleton et al., 2012a). 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, surface features (mountains, rivers, cities tec.), and estimates of both storage capacity and injectivity for specific reservoirs (Middleton et al., 2012b). 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.

Results and Discussion

Quarterly Task 1 involves collaboration between LANL and the Indiana Geological Survey (IGS) to create a system model for CCUS around Duke Energy's Gibson power plant in southern Indiana. A set of 15 nodes within an 80 km circle around Gibson were chosen. These 15 nodes represent a range of both shallow resources (ECBM, EOR, and shale gas) and deeper saline formations (St. Peter, Knox, and Mount Simon). IGS has extended their earlier characterization

work in the Gibson area (Ellett et al., 2013) and completed regional-scale analysis of saline formations and utilization components including ECBM, Shale gas, and EOR. Figures below show the 15 nodes, resources, and analysis of the saline formations.

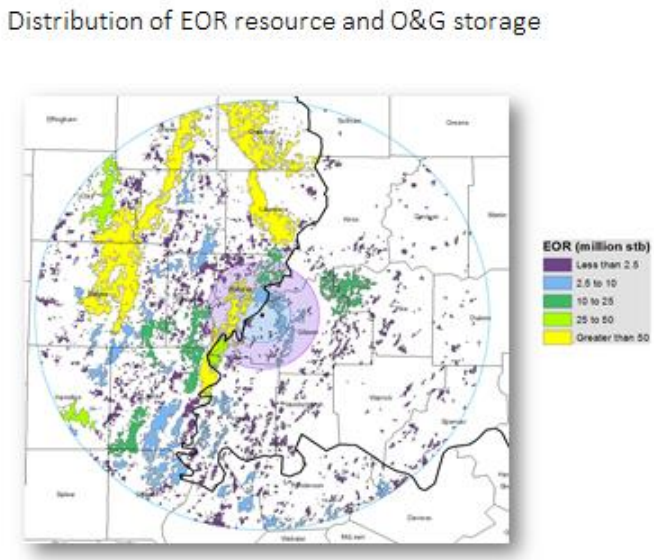

Figure 6.4.B.1-1 Distribution of EOR resources near the Gibson power plant. The purple circle is our 80 km radius of interest for the initial analysis.

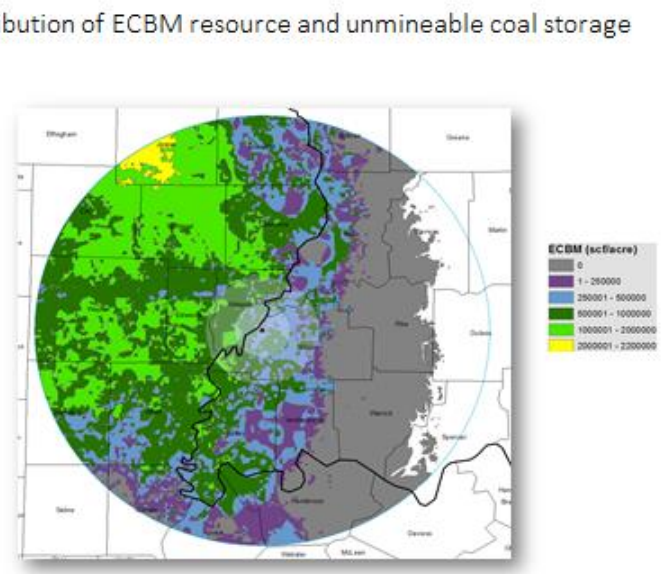

Figure 6.4.B.1-2 Distribution of ECBM resources in the same region

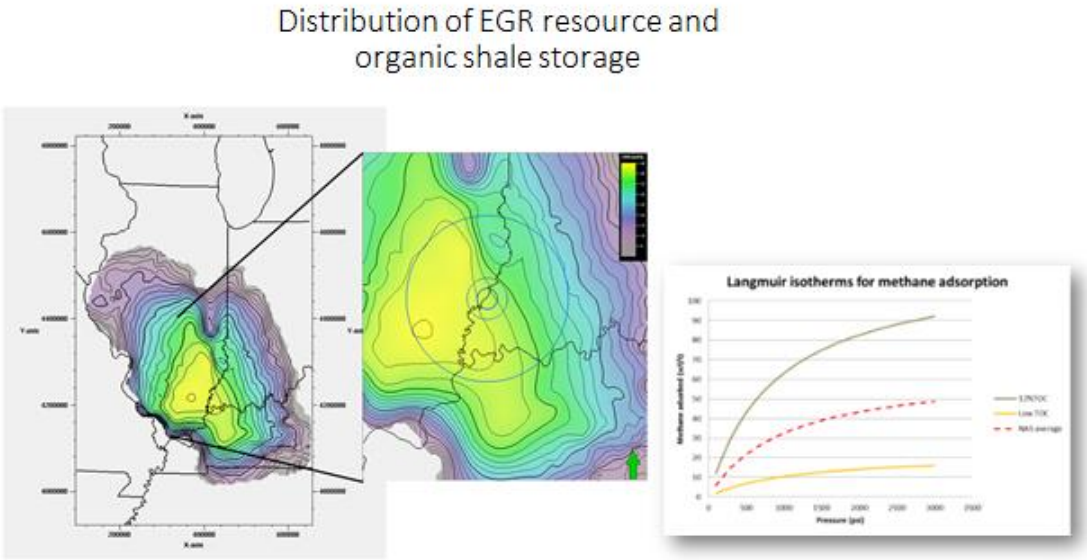

Figure 6.4.B.1-3 Distribution of EGR near Gibson

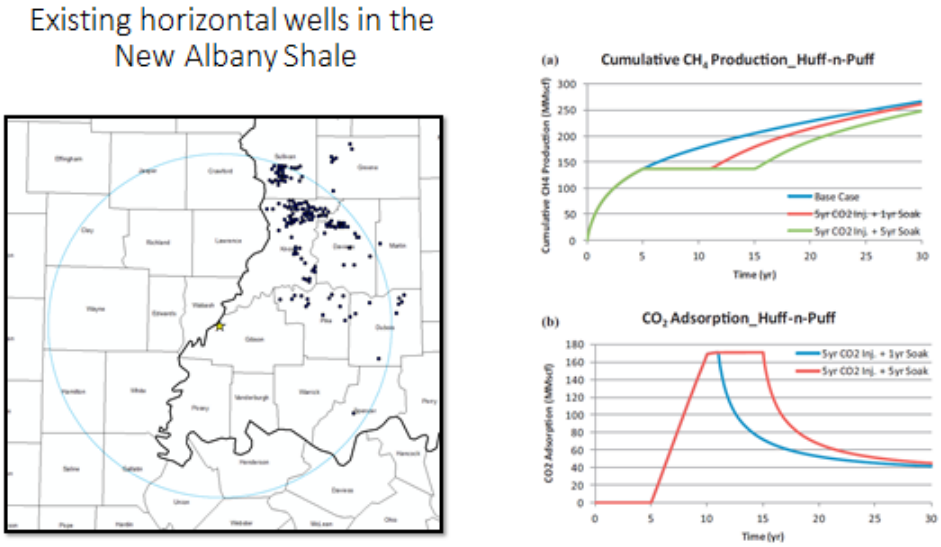

Figure 6.4.B.1-4 Existing shale gas wells in the Gibson area and reservoir modeling results from Liu et al. (2013) to be used for the EGR and shale storage simulations.

Mount Simon reservoir (a) top structure, (b) thickness, and (c) background storage resource model (weighted combination of multiple deterministic models)

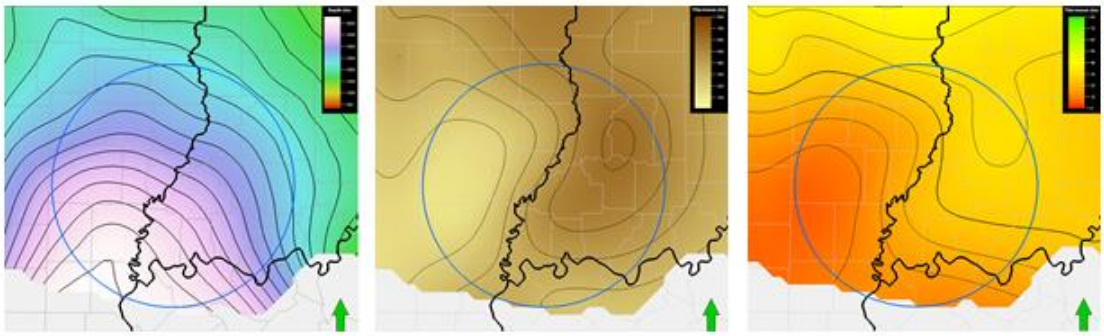

Figure 6.4.B.1-5 Mount Simon saline storage analysis in the Gibson region

Knox Group reservoir (a) top structure, (b) thickness, and (c) background storage resource model (note porosity meter scale is 2X the Mount Simon in prior fig.)

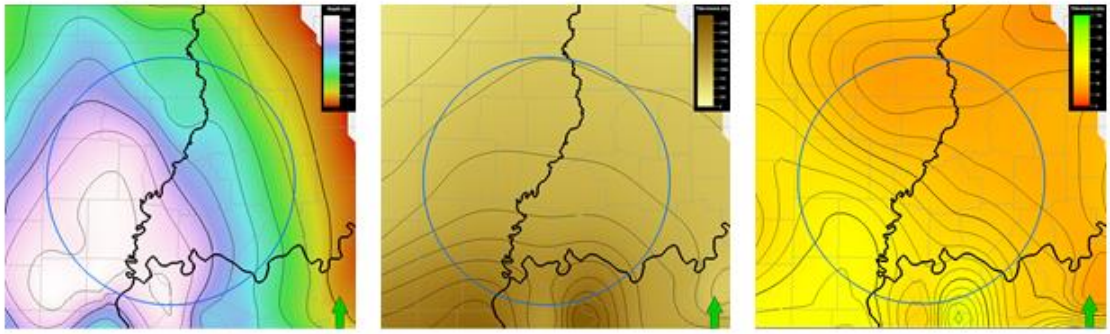

Figure 6.4.B.1-6 Knox Group saline storage analysis in the Gibson region

St Peter reservoir (a) top structure, (b) thickness (note Mount Simon max is 10X larger and Knox Group max is 30X larger), and (c) background storage resource model (note porosity meter scale is order of magnitude less than MTSMN or KNOX)

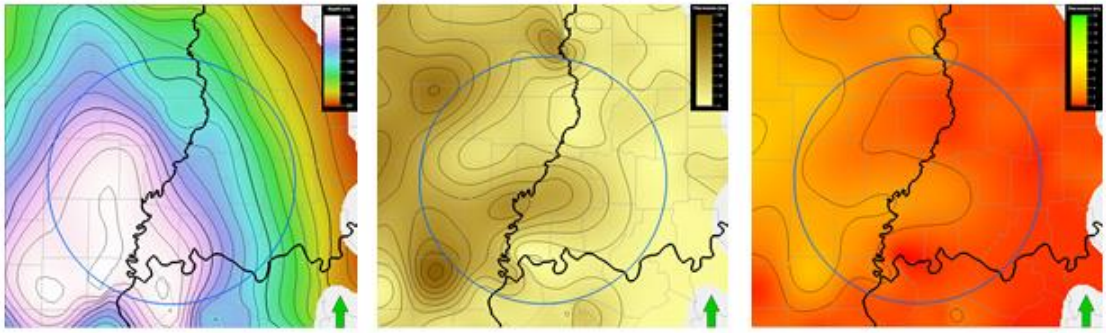

Figure 6.4.B.1-7 St. Peter saline storage analysis in the Gibson region

Porosity-permeability transform equations

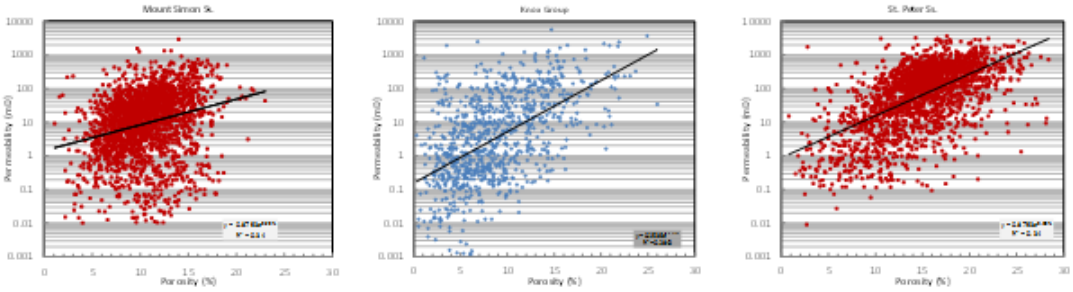

Figure 6.4.B.1-8 Porosity-permeability data for the saline formations of interest

Selection of nodal locations for integrated system modeling with stacked reservoirs/utilization resources (saline formations, EOR, ECBM, EGR)

Node	location	utmX	utmY	SF-MTSMN	SF-KNOX	SF-STPTR	EOR/O&G	ECBM/UC	EGR/NAS
1	On site at Gibson Station	433093	4247026	10	6	26	10	0.4	
2	Clay, IL	384900	4276700	13	6	26	109	1	
3	Tri County	454500	4306500	9	8	54	2	0.2	
4	Lawrence, IL	435800	4283800	10	7	45	48	1	
5	Crawford, IL	432700	4310500	9	8	37	64	0.5	
6	White, IL	410400	4225000	12	5	23	51	1	
7	Pike, IN	463000	4258500	9	7	35	15		
8	Knox, IN	473500	4298500	8	7	43			16
9	Sullivan, IN	460600	4318900	8	8	45		0.25	12
10	Clay-Sailor, IL	378900	4295500	12	6	23	18	1	
11	Wabash, IL	422600	4248700	11	6	26	43	1	
12	Hamilton, IL	365800	4209500	18	5	21	28	0.4	
13	Posey, IN	418500	4214000	11	5	32	3	0.5	
14	Henderson, KY	440600	4168800	13	5	45	12	0.25	
15	Davies, KY	476600	4182500	12	5	51	2		

Color codes: relative resource level– high resource med resource low resource

SF number is the estimated radius of idealized CO_2 plume (km) for 90 million tonne injection using P_{50} estimate of storage resource (tonnes/km^2)

EOR/O&G number is low range estimate of EOR (million stb) for fields in vicinity of node (<5 km). Note that this is larger than the hard dip radius value in Ellett et al., 2013, CERC-JM poster

ECBM/UC number is low range estimate of ECBM (million scf/acre) for unmineable coals in vicinity of node

EGR/NAS number is estimate of gas production (Bcf) assuming huff-n-puff scenario from Liu et al. (260 MMscf cum production and 40 MMscf CO_2 storage) with existing NAS horizontal wells in Knox and Sullivan fields

Figure 6.4.B.1-9 15 nodes located within an 80 km radius of Gibson showing relative saline storage and utilization potential calculated from static geological models.

Map showing selection of nodal locations for system modeling (red stars with 5km radius) along with estimated EOR potential of oil fields and existing horizontal well infrastructure in the New Albany Shale play (blue circles)

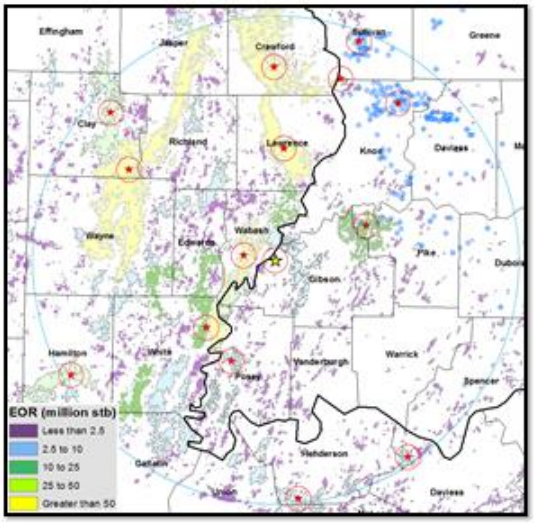

Figure 6.4.B.1-10 Map view of the 15 nodes located within an 80 km radius of Gibson.

The latest modifications to a joint Action Plan for data sharing and analysis on the Ordos and Illinois basins between the CAS, LANL, and the Indiana Geological Survey are shown in appendix I to this report.

The sequestration team is involved in planning a meeting in Wuhan with our Theme 6 Chinese collaborators from both the Chinese Academy of Sciences and the Northwest University. We are

attempting to bring together the Ordos Basin characterization efforts of both of the Chinese teams through an example of characterization and simulation for the Gibson region of the Illinois basin (Quarterly Task 1 above). We continue to work on the Gibson region model and plan to do hands on work while in Wuhan in early May 2014. The current draft agenda is attached as appendix II to this report.

The team developed a presentation for the DOE CCUS conference in Pittsburgh, to be presented by Sarah Forbes. The subject of this talk is a collaborative effort between US and Chinese ACTC scientists to create the first comprehensive study of what an integrated commercial scale CCUS system could look like in China. We focus on the Ordos Basin, which is slightly larger than New Mexico. The basin has a large number of chemical and power industries found within its perimeter that generate greater than 350 MT of CO2 per year. The basin also has a high capacity to store CO2 in a wide range of target formations including CO2 utilization for EOR and ECBM. In order to develop infrastructure to capture, transport, and store CO2, potential pipeline routes need to be identified in the Ordos Basin. We have developed a weighted-cost surface that allows shortest path algorithms to identify low-cost corridors for pipelines. We also built a CO2 emissions database using 290 individual sources that emit approximately 350 MT of CO2 per year. The Majiagou limestone was selected as the target storage formation in the Ordos. Nine target regions were pre-selected based on analysis completed by the Chinese Academy of Sciences. Injectivity was calculated using CO2-PENS, a reservoir simulation framework developed at Los Alamos National Laboratory (LANL). A total of 30 Gt CO2 storage capacity was identified. The candidate pipeline in the Ordos Basin avoids high cost areas such as population centers and topographically complex terrain, particularly in the southern portion of the Ordos Basin toward the city of Xi'an. Using the SimCCS decision model and on this candidate network, we developed optimized combinations of CCS infrastructure in response to (1) a CO2 capture target amount and (2) a CO2 tax on emissions. Example results show an emissions penalty below $24/tCO2 does not stimulate any CO2 capture; that is, all industries emit their entire CO2 emissions because it is cheaper than capturing. From $24/tCO2 until $52/tCO2, approximately 50 MtCO2/yr is capture system wide from the cheapest sources (e.g., coal to liquid plants). Beyond $52/tCO2, it becomes economical to capture CO2 from coal-fired power plants. Additionally, CERC researchers will participate in the upcoming Greenhouse Gas Technologies conference in Austin Texas. This unrivaled CCUS meeting will showcase our CERC work and collaborations on a number of topics.

Plans for Upcoming Quarter

The team will utilize the action plan (attached as an appendix) to guide the work in the next two years of the project.

Theme 6 plans for the future are ambitious and will depend on sufficient funding being made available to the participants by the CERC. This would to allow both LANL and IGS to expand the initial collaborations with both Duke Energy and the Chinese Academy of Sciences in Wuhan. Similarly, the Carbon Management Institute at the University of Wyoming will be moving to a more advanced stage of simulation and modeling including EOR simulations covering parts of the Ordos Basin that could be made more valuable by enhanced funding. Expanded collaboration will require more intensive data analysis and increasingly complex numerical simulations. Ideally, Theme 6 will have enough resources to create more detailed and accurate simulations of geological sequestration that would include incorporating reservoir heterogeneities and site specific structures for both the Ordos and Illinois basins. Additional simulations would also include conceptualizing "carbon utilization" strategies such as

advanced EOR and shale gas simulations which would leverage faculty at the Indiana Geological Survey, Indiana University and University of Wyoming.

1) We will continue work on the Gibson region in collaboration with the Indiana Geological Survey and LLNL. The plan is to incorporate data from subsurface sinks in the Mt. Simon, the Knox, and the St. Peter formations as well as potential EOR sinks in the area surrounding the Gibson site and use this information to address both subsurface risk and regional CCUS risk. An interesting discussion from this collaboration concerns the use of enhanced coal bed methane and/or deep shale as potential sinks for CO_2 in the southern Indiana region. Even preliminary work in this area would greatly assist in the development of Theme 6.3. At the beginning of July, 2013, IGS provided LANL with data on the New Albany Shale, a development that improves our changes of incorporating shale gas production coupled to CO_2 storage into an upcoming techno-economic analysis of the Gibson area. Duke Energy has expressed interest in this analysis and we will present this work in May during our Joint Meeting in Wuhan. Following the Wuhan workshop, we intend to make another presentation on updated system modeling results to our Duke Energy partners within the CERC.

2) LANL continues to work with LLNL and has received the CERC developed geological models of the Gibson site including numerical meshes created for the project. LANL plans to use the numerical meshes to run simulations in parallel with LLNL to answer additional questions of uncertainty that arise during the collaboration. Three primary members of the CERC Theme 6 (IGS, LLNL, and LANL) are being pulled closely together to generate results for the Gibson site work. John Rupp of the IGS has been discussing the value of the CERC work with Duke Energy, Michael Reid and Doug Durst are the principle contacts. After we deliver our initial analysis by May 2014, Duke will be in a better position to engage in the Theme 6 work and will hopefully help guide calculations that would be useful for their long term interests in the region, especially with respect to the regional analysis and the role that EOR may play in the future of CCUS.

3) Discussion with IGS has led to consideration of the Gibson site as a candidate for information sharing with our Chinese Collaborators. Such information sharing was enthusiastically discussed in Xi'an by delegates from both nations, and success in this effort has led to a better working relationship between modelers on the international front. We are beginning to share data and allow showcasing both US and Chinese computational techniques on a common data set, allowing comparison of results including strengths and weaknesses in competing methods. This will rely on the CERCs ability to release realistic information from the site and will likely require approval from DOE and Duke Energy. Xiochun Li of the CAS responded favorably to our plans at the Jackson meeting and we are now scheduled to have a Joint Workshop in May of 2014 in Wuhan.

4) LANL will work with the University of Wyoming (J. Jaio) to set up simulations of CO_2 injection related to sites in the Ordos Basin. The work will begin with CO_2/brine but migrate to inclusion of an oil phase toward the end of Q4 or the beginning of FY14. Development of the oil phase in FEHM is not being paid for by CERC and we thus do not control the schedule of oil phase completion in the code. The oil phase simulations in FEHM may not be ready until the third quarter of FY14. In the interim, we have been using commercial codes to generate results for EOR fields (Quarterly Task 2 Q3FY13). These results are being extracted and built into a reduced order model for risk analysis.

5) Finally, we plan to write papers summarizing the results of the US China collaboration on the Ordos Basin geological sequestration assessment for both the GHGT-12 meeting and a future journal submission.

Theme 7 – CO_2 Algae BioFixation and Use

Subtask 7.1. – Screening of Algae Strains

Approach

Identifying a strain of algae that will endure, and indeed thrive when fed with flue gas is an important aspect of this project. The ability of algae to grow robustly and quickly will define CO_2 uptake rates while the strain used will also play a role in determining the optimum approach for utilization of the biomass. Hence, this subtask focuses on identifying and culturing optimal summer and winter algae strains to be used in the CO_2 mitigation system.

Results and Discussion

In the past quarter, culturing of winter strain *Chloromonas rosae var. psychrophila* was continued in airlift bioreactors. This is a fast growing strain which looks very promising for cold weather cultivation. For harvesting, various types and concentrations of flocculants were used to flock algae. After multiple attempts, flocculant Zinkan 440 at a concentration of 30 ppm worked the best with a culture density close to 1 g/L (dry weight). Algae floc settled to the bottle of the harvest reservoir with a semi-clear supernate lying on top.

Protein analysis of the harvested dried algae indicated a relatively high protein content of 36.85 wt% (+/- 1.78 wt%, based on two measurements). Attempts to determine the sugar content proved inconclusive, so this measurement will be performed again.

Plans for Upcoming Quarter

On-going analysis of *Chloromonas* for lipid, protein and sugar content will be completed.

Subtask 7.2. – Growth System Optimization

Approach

Optimize 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. Specific actions will include working with Duke Energy to identify a site for the pilot-scale demonstration, operation of the demonstration plant using optimal summer and winter microalgae, examining the feasibility of recycling nutrients derived from the anaerobic digestion of algae, and examining the effect of recycle water (derived from harvesting) on algal growth.

Results and Discussion

During the last quarter efforts were focused on prototyping a new photobioreactor design which incorporates cost reduction measures. A new reactor configuration was developed to make more efficient use of sunlight, and thereby capital cost. This staggered row configuration is shown in Figure 7.2.1.

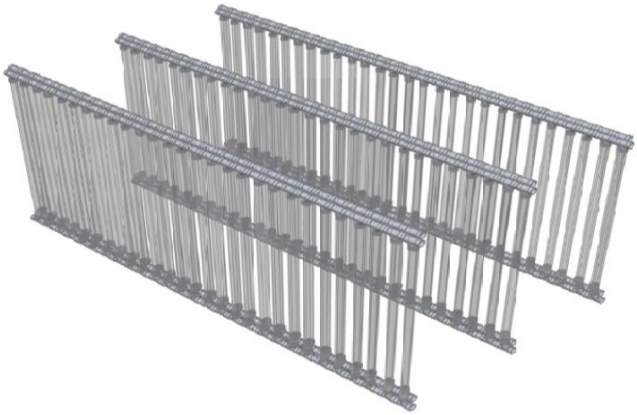

Figure 7.2.1. 3-D rendering of staggered tube design

An 8 tube (~35 gallon) reactor was prototyped and operated to understand how the flow in the system would work. One of the main strengths of this design is its flexibility, offering multiple ways of operation. This new 'cyclic flow' reactor is designed to operate very differently than previous PBR designs. In the past, we have continuously flowed the algae culture though the phototube array which had some unintended consequences. Fully developed flow in a pipe results in a 'no slip' condition at the pipe wall. This provides a convenient space for algae cells to accumulate and reside against the wall of the tube. Given time, these cells will colonize and form a biofilm. The new reactor will not flow continuously and the tubes will instead fill and drain multiple times per day. This will result in flow never being 'fully developed' and should greatly reduce biofilm formation (not having to flow the reactor continuously will also result in an energy saving). Biofilm mitigation will also be tackled by (i) the introduction of gas bubbles in the reactor body to create multi-dimensional fluid mixing, (ii) cycling the flow in order to disrupt the biofilm formation process, and (iii) through the use of a 'pipe pig' to clean the reactor walls as flow is cycled. Figures 7.2.2a and 7.2.2b show the prototype 'cyclic-flow' reactor and an installed prototype pipe pig.

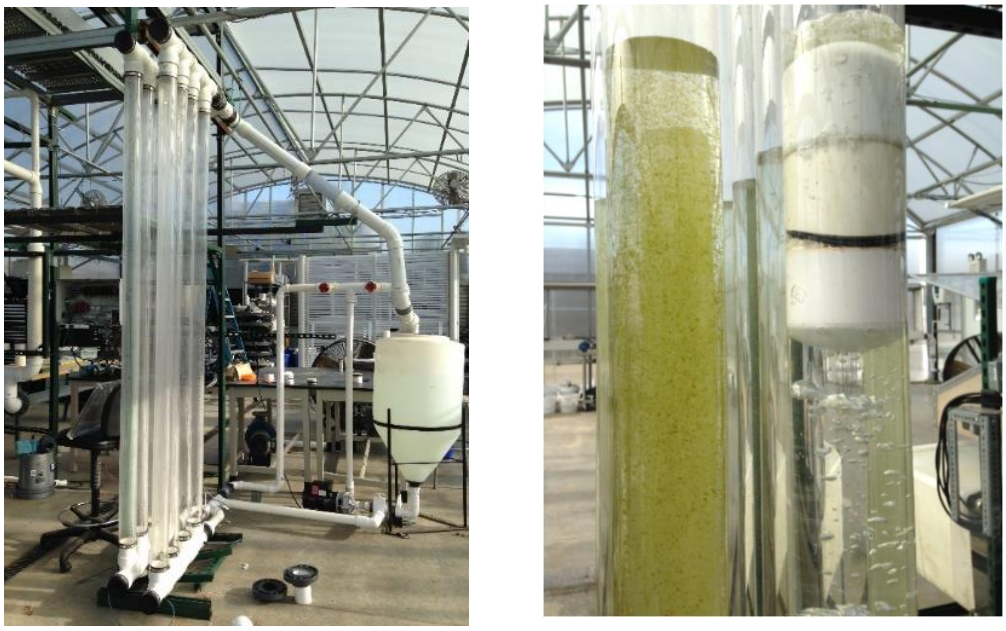

Figure 7.2.2. (a) The 'cyclic-flow' prototype PBR (left) and (b) pipe pig prototype 2.0 (right)

Parts have been ordered to construct a full size prototype in the CAER greenhouse for evaluation. This new design should reduce energy operating costs, increase performance, reduce the capital cost, and improve operational stability to provide a platform for performing accurate mass balances on the process. The plan is to have the new reactor design, incorporating the findings from the student engineering teams (see below) along with other updates, installed at East Bend Station by the time the plant returns from their scheduled spring outage.

Good progress is being made with both electrical and mechanical engineering student design teams who are focused on designing/developing a low cost control system and a low cost frame. Both the teams had critical design reviews for their project, finalized their designs, and have moved into the prototyping phase. The electrical engineers were tasked with designing, building, and testing a control system capable of growing algae. The most important cost reduction measure was the identification of a water chemistry company named Atlas Scientific which provides low cost, durable sensors. Signals from these probes will be fed to a small microprocessor which will process and record the data and control actuators to maintain desired growth conditions in the reactor. Figure 7.2.3 shows a schematic of the control system.

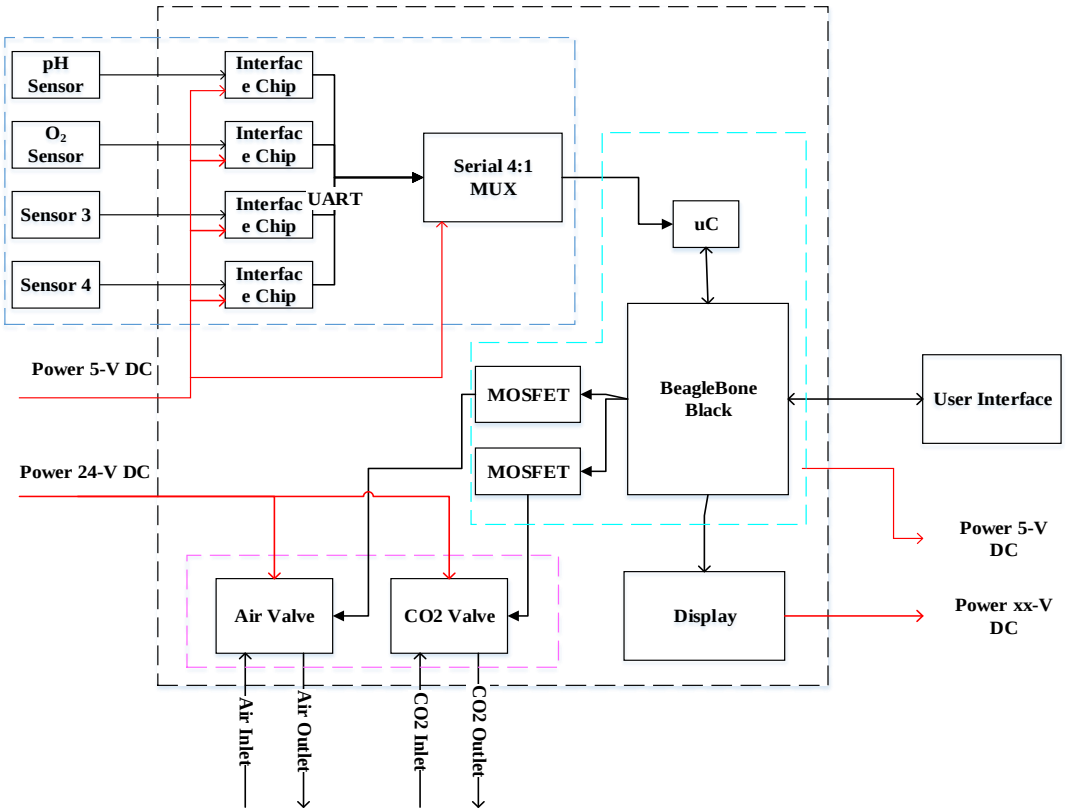

Figure 7.2.3. Control System Diagram

The electrical team has exceeded expectations with respect to their creativity, productivity and professionalism, and we are eager to put the prototype control system through its paces. The team also met its cost reduction target, reducing the control system cost by 50%.

During techno-economic analyses last year, the support frame was identified as an area with significant scope for improvement. A mechanical engineering senior design team was

challenged to reduce the capital cost of the support frame by a factor of three. The team examined a number of creative solutions before settling on a steel frame capable of supporting the weight of the water-based algal culture, as well withstanding forces due to wind. A digital rendering of the final design is shown below in Figure 7.2.4.

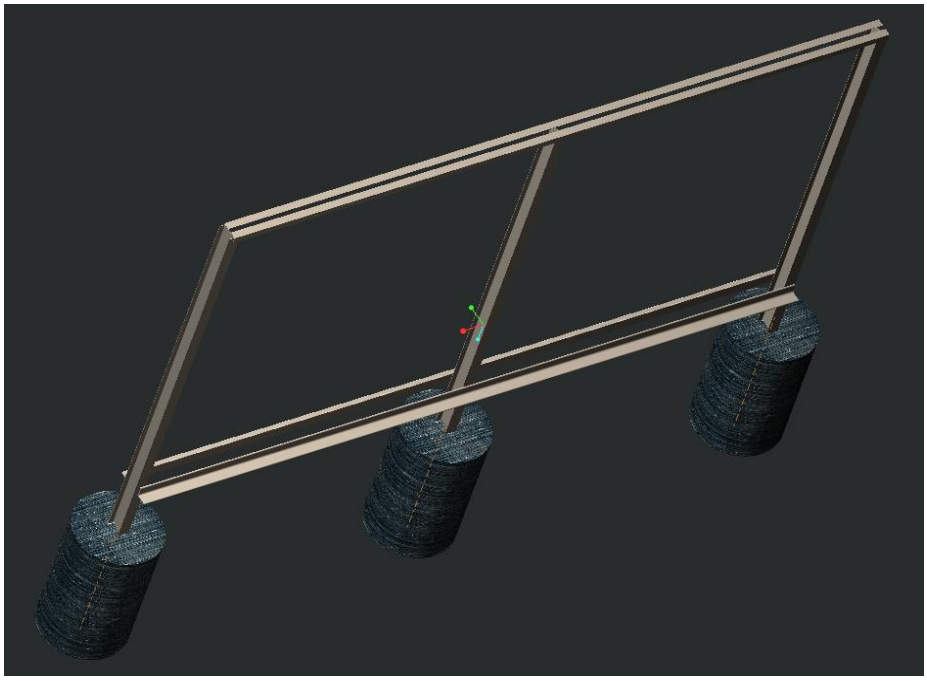

Figure 7.2.4. 3-D model of support frame

The students employed finite element modeling techniques to evaluate the performance and deflection of different designs while trying to minimize material and construction costs. An illustrative analysis of one of the designs is highlighted in Figure 5, which illustrates exaggerated deflection of the photobioreactor tube array.

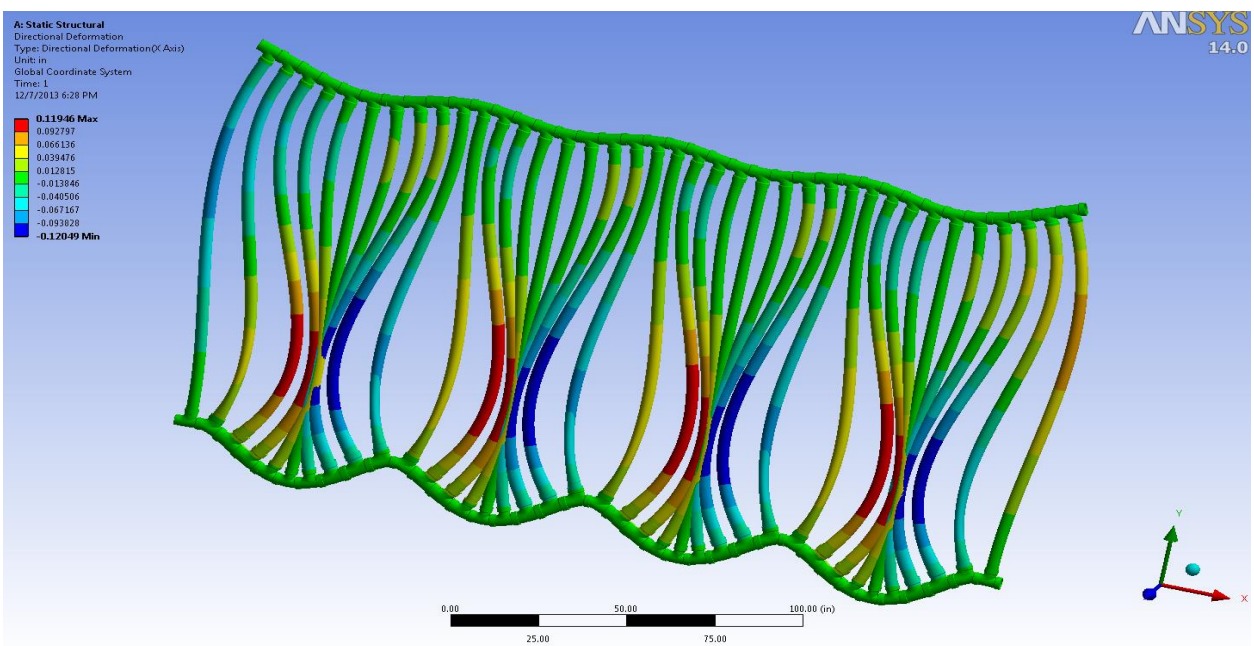

Figure 7.2.5. Results from finite element analysis

The mechanical team has excelled in applying practical engineering analyses to a real world problem and initial cost calculations indicate that they met their 67% cost reduction goal. A prototype frame, modified for installation and use at East Bend, will be constructed at the UK CAER and tested before the frame is scaled up and built on site.

Plans for Upcoming Quarter

Efforts will continue to scale up and test the photobioreactor in preparation for deployment at East Bend. A cheaper alternative to the pipe pig will be designed and prototyped. Work with the student design teams will wrap up and their prototypes will be tested.

Subtask 7.3. – Algae Post Processing

Approach

When using microalgae to biologically fix CO_2 contained in flue gas (in essence, enabling the CO_2 to be recycled), there is the potential to obtain valuable biomass-derived products which can help to off-set the high costs of algae cultivation and processing. To this end, this subtask aims to assess the various products (and their corresponding value) which can be derived from algal biomass.

Results and Discussion

Very recently experiments were initiated to optimize our method for lipid extraction from wet (as-harvested algae). This incorporates the use of a water-miscible solvent (THF), followed by the use of an inexpensive, acidic adsorbent to remove the chlorophyll present. Work is being performed by a visiting foreign exchange student (from France) and a high school student. Initial results will be presented in the next quarterly report.

Plans for Upcoming Quarter

Work on lipid extraction and purification will continue. New lipid upgrading experiments for the production of diesel-range hydrocarbons (based on catalytic decarboxylation/decarbonylation) are also planned.

Subtask 7.4. – Techno-economic Analysis

Approach

We plan to leverage the expertise of the US and Chinese project partners to conduct a detailed techno-economic assessment of the potential of algae for CO_2 utilization. Working with Duke Energy, biological CO_2 fixation at a coal-fired power plant will be demonstrated, the resulting data functioning as inputs for the techno-economic model. In this manner, we aim to arrive at rational and detailed cost estimates for CO_2 fixation and utilization.

Results and Discussion

No work was performed on this task in the last quarter.

Plans for Upcoming Quarter

Work will begin on a lifecycle analysis of CO_2 capture and recycling using algae, incorporating the improvements made in the refined photobioreactor design.

Theme 8 – Integrated Industrial Process Modeling and Additional Topics

Subtask 8.1: Power Plant Cycling and Load-Following Operations (NEW)

Approach

Coal-fired power plants are experiencing increased cycling and load-following operation for several reasons: demand for electricity from the grid fluctuates over time; natural gas plants supply more baseload power; and, variable renewable and intermittent power generation (e.g., wind, solar) grows more rapidly in the modern grid era.

Many coal-fired plants were not designed to operate with large variations in power output, but must now cope with wide changes in power demand, often on an hourly basis. This increased cycling and load-following operation will degrade plant performance, e.g., increased derates and emissions. In addition, plant stress and equipment damage via thermo-mechanical fatigue will be accelerated and plant operation and maintenance costs will increase.

The purpose of this new, DOE-NETL-lead project will be to investigate the effect of repeated cycling of coal-fired plants by integrating the AVESTAR high-fidelity, real-time dynamic simulators to Intertek's COSTCOM® for use in computing damage accumulation rates and dollar costs for cycling operation and determining the cost impacts of increasing ramp rates, MW load transient ranges, and shortened startup times.The results of this work will improve cycling and ramping strategies to minimize thermal and pressure gradients, reduce costs, minimize damage accumulation rates, and improve control of load transients.

Results and Discussion

No progress this quarter

Plans for Upcoming Quarter

Subtask 8.2: Systems Modeling of Post-Combustion Capture Technology

Approach

Blower Performance Curve

Based on the packing sizing calculation for Intalox™, the pressure-drop through the absorber is very small, 2-3kPa. Similarly, pressure-drop through the direct contact cooling and washing sections can also be calculated. The inlet pressure before the CO_2 capture process is assumed to be 1.133bar by considering the pressure-drop through all equipment and the frictional pressure drop through the connecting piping. From the simulation results of the pulverized coal-fired power plant, flue gas enters the CO_2 capture section at 1.026bar and 57.6°C. Therefore, the desired differntial pressure increase across the blower is about 0.107bar at the design flowrate of flue gas. At steady-state, the flue gas leaves the blower at 1.133bar and 69.9°C. The flue gas volumetric rates at the inlet and outlet of the blower are 563.8 and 532.2 m^3/s, respectively. As CO_2 absorption is sensitive to pressure change and air compression contributes significantly to the auxiliary power loss, a smaller pressure change (thus lower blower differential pressure) is preferred for the CO_2 capture process. The blower was designed to be able to operate under different conditions by changing inlet guide vane (IGV) angle. The performance curve for the blowers used in the current work is shown in Figure 8.2.1.

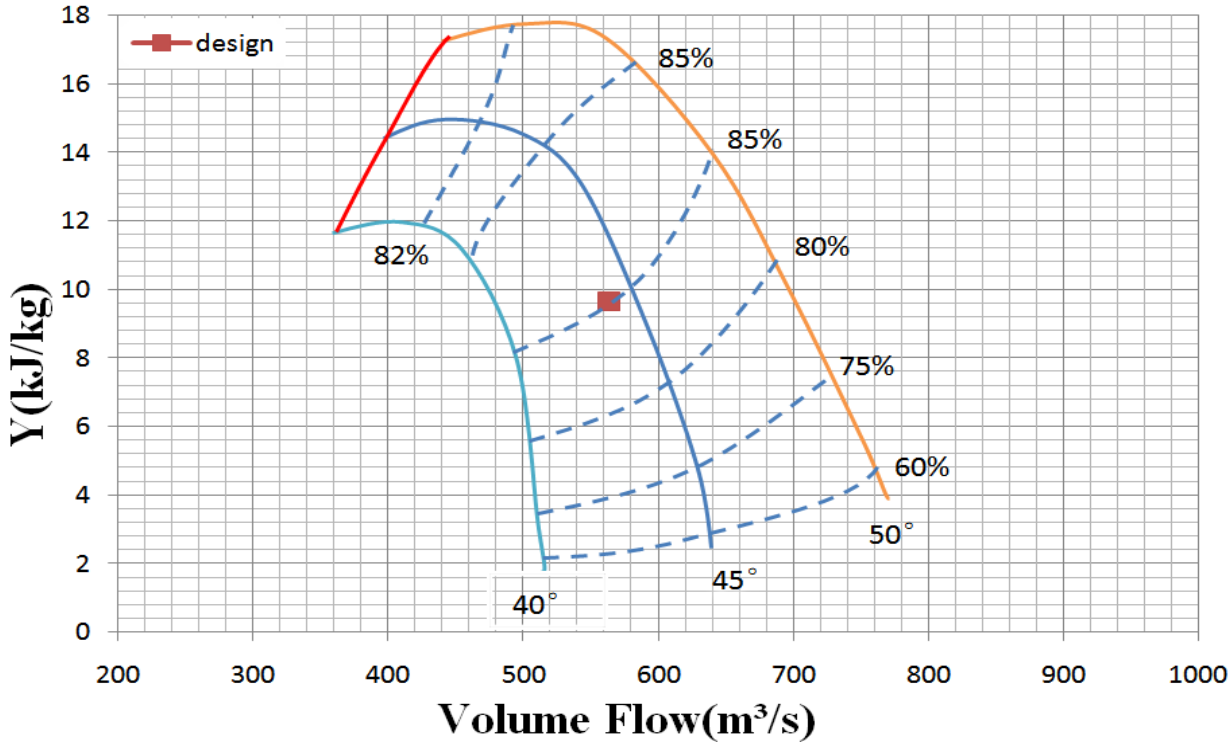

Figure 8.2.1: Designed flue gas blower performance curve

Since IGV angle is not considered as an input for blower in Aspen Plus Dynamics, shaft speed was used to replace the IGV angle for flue gas flow control. The base case design uses a separate blower for each absorber/stripper train. Therefore, the volume flow in Figure 1 was divided by six while keeping the other variables unchanged, in order to get the performance curve for each blower in an individual train.

Separate Reboiler Model

The basic stripper model in Aspen Plus Dynamics has a built-in reboiler and the temperature at last stage is maintained by adjusting the heat duty. However, the heat needed to recover CO_2 and solvent is provided by the extraction steam and the duty is determined by the operating conditions in reboiler. In order to simulate more realistic reboiler transients, a separate reboiler was designed and modeled using the last stage condition of the stripper at steady-state conditions. The reboiler size was determined using the Aspen Exchanger Design and Rating package. A part of the stripper bottom product is heated and partially evaporated in the separate reboiler and returns at the last stage of stripper. The temperature at the last stage in the stripper is maintain by manipulating the flow rate of extraction steam. The flowsheet for the stripper with separate reboiler is shown in Figure 8.2.2.

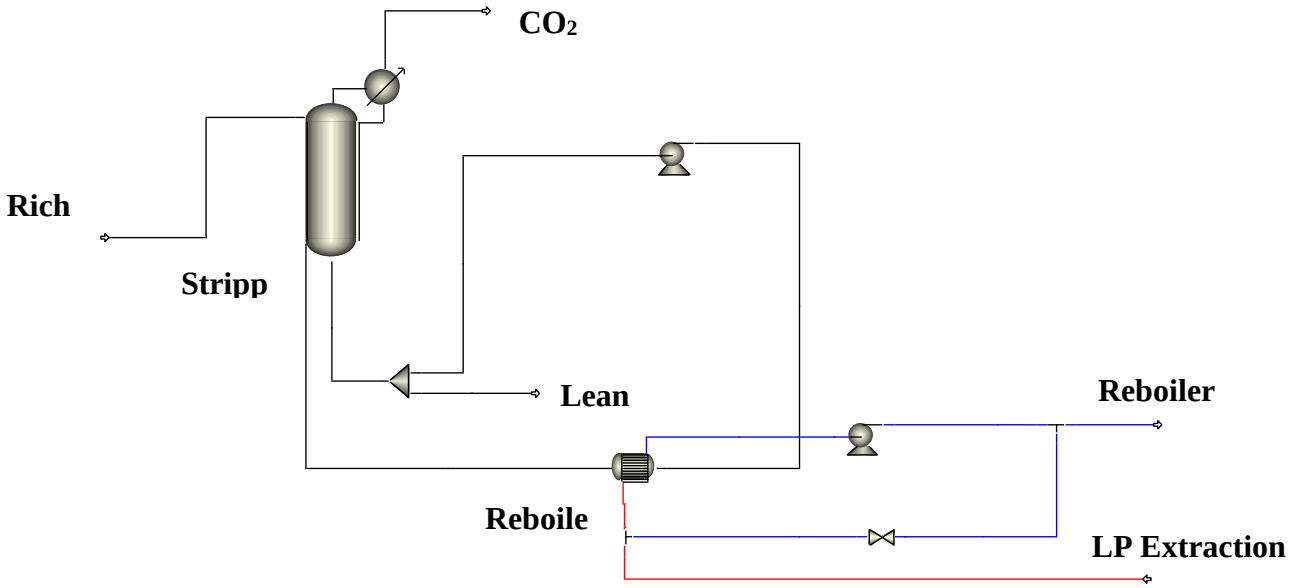

Figure 8.2.2: Flowsheet of stripper with separate reboiler

Simulation Transients

Prior to the design of the control system for the 550MWe supercritical coal-fired power plant with CO_2 capture process, a long-time test on the dynamic simulation was carried out to evaluate the approach to steady-state using a basic PID (proportional-integral-derivative) control strategy. The result showed that this system cannot reach a steady-state because the lean solvent flow rate and stripper last stage temperature keeps fluctuating, as shown in Figures 8.2.3 and 8.2.4. This can be caused by the large solvent inventory within the MEA-based CO_2 capture process and the less efficient temperature control of reboiler. As the temperature at the last stage of the stripper decreases, the CO_2 loading in the lean solvent increases and more solvent will be required to maintain the 90% CO_2 capture rate. Therefore, the solvent circulation rate increases and more rich solvent goes into stripper. This can further lower the stripper temperature because the stripper last stage temperature controller does not foresee the increase in solvent flow rate and take quick action to increase steam extraction flow rate. Controllers with time delay and Model Predictive Control (MPC) would be expected to help eliminate these fluctuations.

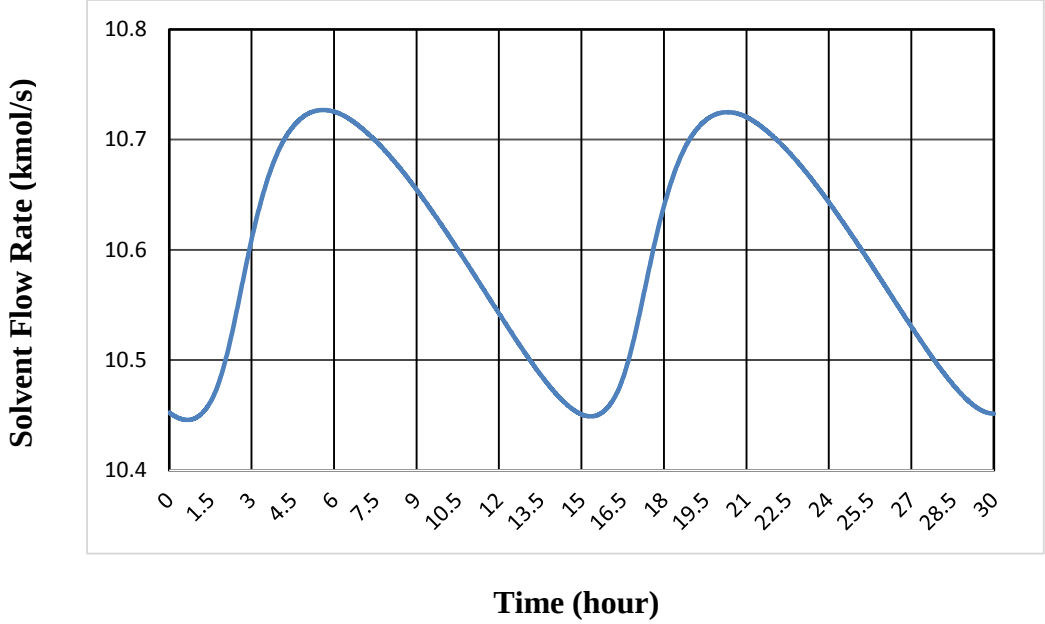

Figure 3: Lean solvent flow rate profile

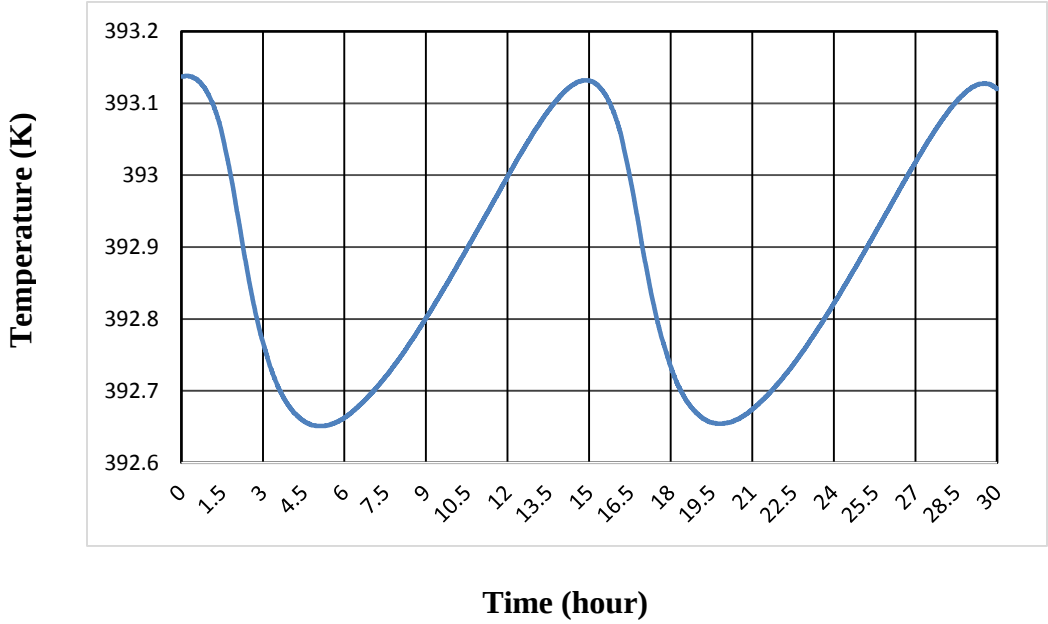

Figure 4: Stripper bottom temperature profile

Other Efforts to Accelerate Dynamic simulation

The Aspen OTS framework provides a platform to run a large dynamic simulation in real time using parallel processing. Current computers usually have two or four processors and one dynamic simulation is only executed on one single processor. With the Aspen OTS framework, a large dynamic simulation can be split into several parts. Streams and control signals connections can be established between different partitions to exchange data. Each partition is a single smaller dynamic simulation and Aspen OTS framework will assign different partitions into different processors. Therefore, the large dynamic simulation is accelerated. However, a critical

issue was found when applying Aspen OTS framework to the integrated dynamic model. When all the partitions are set to be pressure-driven, the data could not be exchanged and an action in one partition has no effect on the other connected partitions. The sample used to demonstrate Aspen OTS framework is developed in Aspen HYSYS, which is a dynamic simulator different from Aspen Plus Dynamics and is not applicable to the current work.

Plans for Upcoming Quarter

- Continue to work on accelerating the dynamic model.
- Repeat the system identification proicess based on the integrated dynamic model.
- Apply Model Predictive Control (MPC) to the integrated dynamic model.

Subtask 8.3: Initialization of Dynamic Model with Immersive Visualization

Approach

Initialization and augmentation of a dynamic model with immersive visualization capability for a generic IGCC system with gas turbine and steam bottoming cycle is addressed in this subtask. NETL and WVU have dynamic models and an operator training facility for a generic IGCC coal-fed power plant and the implementation of a 3D immersive training system (ITS) is planned. We propose to offer training to our Chinese collaborators through the CERC project and funds to cover this training are included in the WVU budget.

Results and Discussion

No Activity this quarter

Plans for Upcoming Quarter

No input.

Subtask 8.4: Static and dynamic modeling of post combustion carbon capture plant; tools for training and visualization

Approach

Static and dynamic modeling of post combustion carbon capture plant; tools for training and visualization.

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 8.5: Modeling of pre-combustion process and IGCC commercial knowledge exchange

Approach

Modeling of pre-combustion process, IGCC commercial knowledge exchange; solvent-based commercial assessment; static modeling of new technologies; static modeling of pulverized coal boiler power plants with carbon capture; tools for training and visualization.

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Subtask 8.6: Life-cycle analysis of coal-to-chemical systems with pre-combustion capture. **(**Shenhua group**)**

Approach

China Supported Task Only. Does not include DOE or Cost Shared Support. Any technical data or results provided to the US CERC-ACTC Team will be included in project reporting. Task is included for completeness and clarity.

Results and Discussion

No input.

Plans for Upcoming Quarter

No input.

Theme 9 – Communication, Integration, and Intellectual Property Rights Management

Subtask 9.1. – International communications and integration support.

Approach

The CERC ACTC strives to operate as an integrated bilateral team working together on research designed to benefit both countries. The complexity naturally rising from the multi-partner and multitask effort makes it necessary to have efficient and effective communication among the teams and tasks to promote successful collaboration and integrate the research progress of different tasks. The primary goals of the theme are three-fold:

- Ensure effective sharing of information and facilities.
- Facilitate personnel exchanges among the different teams of the two countries and the different tasks of the consortium.
- Establish a communication network inside the US-China consortium to maximize the achievements of the cooperation. This includes integration other technical tasks within each national team as well as international coordination.

Results and Discussion

- Coordinated and engaged with meetings for the US and China ACTC partners, e.g. the meeting of University of Kentucky, Tshinghua, Huaneng in January, 2014
- Organized meetings for the US Department of Energy with China ACTC leaders in Tshinghua University in Febrary, 2014
- Participated in China-side ACTC leadership meeting on March 1, 2014; plan to attend China's ACTC Annual meeting on April 21, 2014
- Coodinating with the China-side ACTC leadership to prepare the US-China Annual Metting in September, 2014
- Coordinating with Chinese and US theme leaders for CERC 2.0 Collboaration Plan

Plans for Upcoming Quarter

- Continuing communicating between the US and Chinese ACTC Theme leaders to further develop CERC 2.0 Collboaration Plan
- Participating in ACTC Sequestration Bilateral Workshop in Wuhan, May 4-10

Subtask 9.1. – International Standards Development (ISO TC265).

Approach

WRI is engaged as a liaison to the development of international standards for CCS (ISO TC265). Sarah Forbes is also a member of the US Technical Advisory Group (US TAG) and has been appointed to Workging Group 5 (WG5), Cross Cutting Issues. The ISO TC 265 is chaired by Canada with China as the mirror chair.

Results and Discussion

During this quarter ISO TC265 met in Berlin (March 31-April 3, 2014). Sarah Forbes and LI Xiaochun (CAS) presented a joint proposal first to WG5 and then to the ISO TC265 plenary on a

proposal for new work on the overall risks associated with integrated CCS projects. The proposal will be put to a vote in the coming months and prior to the next plenary.

Plans for Upcoming Quarter

The team will continue working with CAS on developing and building support for the ISO TC265 risk assessment proposal. This includes participation in the upcoming Wuhan Theme 6 workshop.

The US-China teams

The current membership of the ACTC teams in the US and China are summarized in Tables 9.1.1 and 9.1.2. Members include research institutions, universities, national labs, NGO, and companies with long and successful partnerships working with both sides.

Table 9.1.1. The US-ACTC CERC team

Consortium Director: Dr. Jerald J. Fletcher, West Virginia University			
Technical Program Lead: TBD (In process now)			
Universities and Geological Surveys	**National Labs**	**Non-governmental organizations**	**US Companies**
West Virginia U.	Lawrence Livermore Natl. Lab	US-China Clean Energy Forum	LP Amina
U. of Wyoming	Los Alamos Natl. Lab	World Resource Inst.	Duke Energy, Inc.
U. of Kentucky	National Energy Tech. Lab		
Indiana Geol. Survey			
Washington University at St. Louis			

Table 9.1.2. The China-ACTC CERC team

Consortium Director: Dr. Zheng Chuguang, Huazhong University of Science and Technology Dr. Xu Shisen, Huaneng Clean Energy Research Institute		
Chief Scientist: Yao Qiang		
Research Institutions	**Universities**	**China Companies**
Huaneng Clean Energy Research Institute	Huazhong U. of Science and Technology	China Huaneng Group
Research Center for Clean Energy and Power, Chinese Academy of Sciences	Tsinghua U.	Shenhua Group
Institute of Rock and Soil Mechanics, Chinese Academy of Science	Zhejiang U.	ENN
Shaanxi Provincial Institute of Energy Resources and Chemical Engineering	China U. of Mining and Technology	China Power Investment Corp. Group
Northwest University	Shanghai Jiao Tong U.	China Power Engineering Consulting Corp.
	Harbin Institute of Technology	Shaanxi Yanchang Petroleum (Group) Co., LTD.
	Northwest U.	Gemeng ** (Pending)

Summary

Figure 9.1.1 provides a summary of the specific research projects being conducted under each research theme and indicates the nature of the collaboration on that project. In total the CERC ACTC includes 38 projects, 32 of which are joint, 5 of which are crosscutting and 6 of which are conducted by either the US or China to compliment CERC ACTC research.

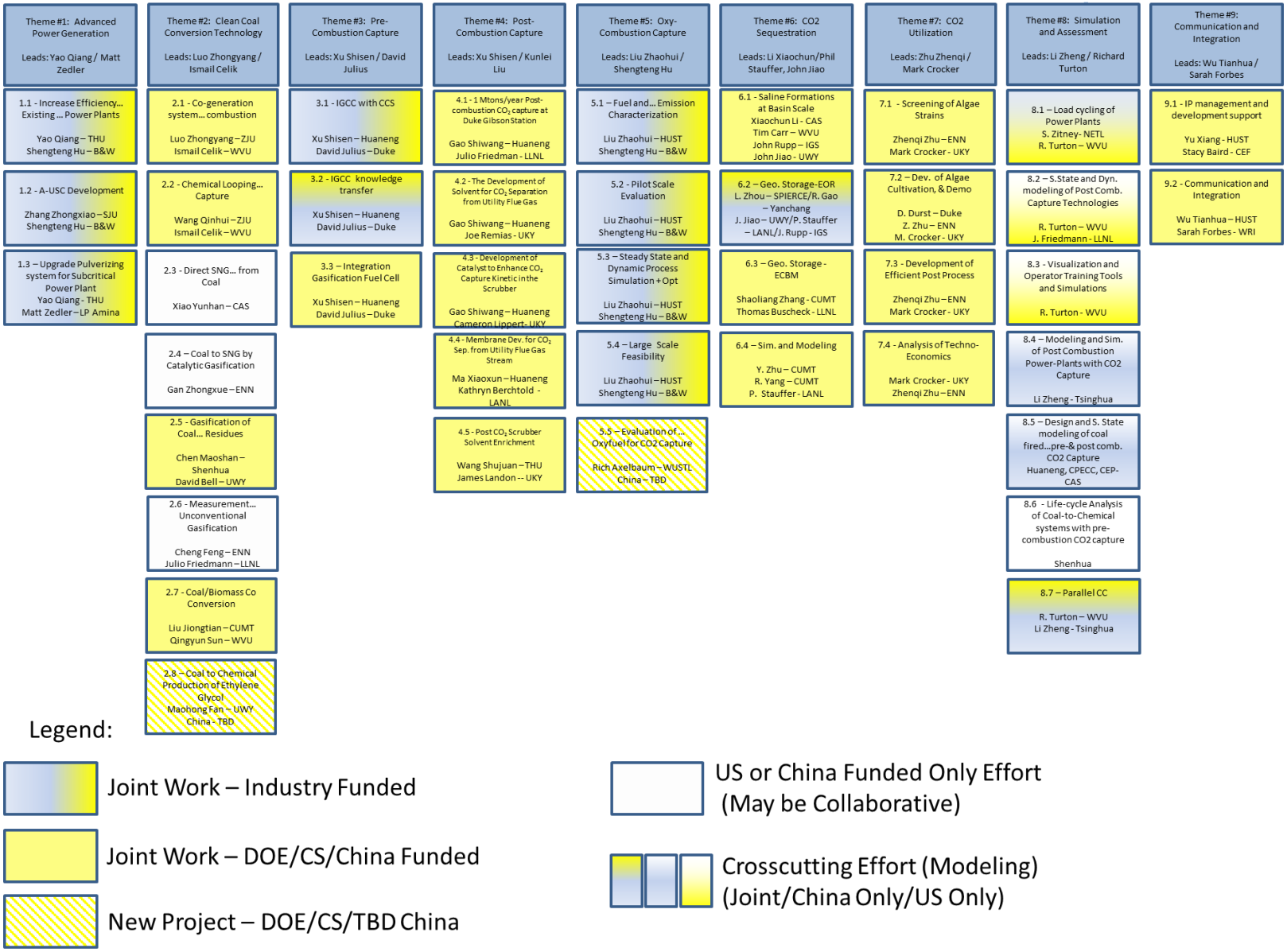

Figure 9.1.1. CERC-ACTC Project Listing

Subtask 9.2. – IP Management and Development Support

Subtask 9.2 – Intellectual Property Management and Support

Approach

The US-China Clean Energy Forum (CEF) recognized a "toolbox" of resources should be developed to help researchers implement the IP aspects of the CERC Protocol, its IP Annex and the Technology Management Plans (TMPs). This "toolbox," would include several guidance and instructional documents which we have described in previous quarterly reports. CERC leadership also recognized the value of an IP Workshop to educate participants with regard to CERC IP, the TMP and applicable laws of each country. In March, during the course of the first IP Workshop, it was recognized that additional work products would be valuable for CERC researchers, including assembling the bilingual presentations from the March 2012 IP Workshop, creating a report on the first IP workshop which may serve as guidance to researchers and developing answers to researchers "Frequently Asked Questions." A second IP Workshop was to be planned for the fourth quarter of 2012 or first quarter of 2013. Finally, in the first two years of the CERC, it became apparent that IP is a central area of interest and concern for CERC Participants. For this reason, CERC leadership evaluated whether to establish a working group to address IP issues going forward. In its initial conception, along with the other two consortia, CERC ACTC would provide expertise and support for such a working group.

Results and Discussion

No activity reported this quarter.

Subtask 9.2.1 – Intellectual Property Workshops

Approach

Following the success of the first IP Workshop held in Hainan, China in March, 2012, the second workshop took place February 26-27, 2013 at Stanford Law School in Palo Alto, California. CEF was responsible for organizing the Workshop for the US.

Results and Discussion

No activity reported this quarter.

Plans for Upcoming Quarter

Subtask 9.2.2 – Technical Assistance and Guidance Documents

Approach

As an outcome of the first IP Workshop, CEF has taken the lead in developing support materials and continue to provide Participants general technical support with regard to intellectual property issues arising with regard to CERC projects and in CERC-related contract negotiations.

Results and Discussion

No activity reported this quarter.

Plans for Upcoming Quarter

Subtask 9.2.3 – Bilateral Intellectual Property Working Group

Approach

From the initial observations that IP was of central concern and interest for CERC Participants, interest grew among all CERC consortia to establish an IP Working Group. Last quarter, US and China's CERC leadership agreed to establish a joint US-China Intellectual Property Experts Group to identify and implement approaches to enhance innovation, utilization, protection and management of intellectual property, for CERC and oversee the provision of technical assistance with regard to IP for CERC Participants.

The US-China CERC IP Experts Group will explore such ideas as new approaches to dispute resolution to minimize litigation risk and reduce the cost of disputes, such as alternative dispute resolution undertaken in a third-party country, under internationally accepted rules and enforced by both the U.S. and China, mechanisms to establish damages awards or injunctive relief, intellectual property risk insurance and other approaches to clarify legal relations of IP ownership and sharing between the project partners, to safeguard the legitimate interests of the partners, and to promote research and development and commercialization.

The Experts Group will oversee other initiatives to provide IP related services to CERC participants which could include executive training, researcher education on IP or consulting or negotiation facilitation services to CERC projects.

Results and Discussion

No activity reported this quarter.

Plans for Upcoming Quarter

Subtask 9.2.4 – Consistent and Transparent Process to Bring New Participants into CERC

Approach

CEF identified a need to ensure there is a clear pathway and transparent uniform process to bring new business, industrial and non-governmental entities into one or more of the CERC consortia as participants. It was determined by CERC leadership that there would be an agreement between DOE and MOST that would describe the basic requirements and process for consortia inviting an entity to join CERC.

Results and Discussion

No activity reported this quarter.

Plans for Upcoming Quarter

Theme 0 – Project Management Activities

Subtask 0.1. – Hold relevant meetings and teleconferences

Approach

Results and Discussion

During the current reporting quarter, the US CERC-ACTC team held a technical meeting with Technology Managers and Project Managers of the National Energy Technology/Fossil Energy program office. The purpose of these meetings was to identify possible avenues for technical work in future years, to communicate the progress and content of the research to the NETL team, and to generally identify potential synergies and opportunities for work with the DOE Fossil Energy Research Program.

Plans for Upcoming Quarter

Subtask 0.2. – Appoint and Manage Private Sector and Technical Advisory Boards

Approach

The initial Private Sector Advisory Board (PSAB) was composed of industrial partners identified in the original proposal.

Results and Discussion

The ACTC team continues to outreach to other relevant Private Sector entities, and will continue to work add team members of high value to the program. The Private Sector Board continues to meet monthly with the project team to discuss project direction and research topics.

Plans for Upcoming Quarter

Continue to outreach to private sector entities, with a renewed focus on US industrial partners.

Subtask 0.3. – Create a commercialization plan

Approach

A Technology Management Plan (TMP) will be created to manage intellectual property provisions and sharing for organizations partnered under the CERC-ACTC.

Results and Discussion

No activity this quarter.

Plans for Upcoming Quarter

No input.

Subtask 0.4. – Manage and update Web site

Approach

A SharePoint site was developed for effective transfer of information between the internal and external stakeholders.

Results and Discussion

No activity this quarter.

Plans for Upcoming Quarter

No input.

Subtask 0.5. – Hold end-of-year meeting and publish report

Approach

The Directors of the US ACTC and the China ACTC (approved by Bob Marlay, the US CERC Director) have an agreement to develop a report for joint activities through December 31, 2013.

Results and Discussion

The annual report is near completion. The project report was jointly developed similar to last years report.

Plans for Upcoming Quarter

Subtask 0.6. – Maintain and update management systems and procedures

Approach

Results and Discussion

Work continues to maintain the integrated and detailed Program plan, including information on budget and technical progress. Plan has been updated to include progress in FY13, and to baseline plans for FY14.

Plans for Upcoming Quarter

Work is ongoing with members of the US and Chinese ACTCs to develop outyear/future work plans. Project plan will continue to be maintained throughout the fourth project year.

Subtask 0.7. – Facilitate Research Exchanges

Approach

Results and Discussion

As outlined in the individual sections of this report, the technical teams continue to host technical exchanges.

Plans for Upcoming Quarter

Theme 6 plans a significant research exchange in the July timeframe. More details are included in the Theme 6 appendix and technical section.

Subtask 0.8. – Communicate the Outcomes of the Research

Approach

Publish results of research in the peer-reviewed literature and presentations at technical conferences.

Results and Discussion

The annual report is near completion. The project report was jointly developed similar to last years report.

Plans for Upcoming Quarter

Cost Status

Project Title:	US-China Clean Energy Research Center Advanced Coal Technology Collaboration
DOE Award Number:	DE-PI0000017

YEARS 1-7 Start: 10/01/10 End: 09/30/2015

Baseline Reporting Quarter	Q1 (12/31/10)	Q2 (3/31/11)	Q3 (6/30/11)	Q4 (9/30/11)	Q5 (12/31/11)
Baseline Cost Plan	(From 424A, Sec. D)				
(from SF-424A)					
Federal Share	2,500,000				5,000,000
Non-Federal Share	2,711,000				5,422,000
Total Planned (Federal and Non-Federal)	5,211,000				10,422,000
Cumulative Baseline Costs					
Actual Incurred Costs					
Federal Share	0.00	366,506.38	460,573.82	677,725.95	516,169.87
Non-Federal Share	0.00	0.00	42,304.06	169,384.07	126,960.28
Total Incurred Costs - Quarterly (Federal and Non-Federal)	0.00	366,506.38	502,877.88	847,110.02	643,130.15
Cumulative Incurred Costs	0.00	366,506.38	869,384.26	1,716,494.28	2,359,624.43
Uncosted					
Federal Share	2,500,000.00	2,133,493.62	1,672,919.80	995,193.85	2,979,023.98
Non-Federal Share	2,711,000.00	2,711,000.00	2,668,695.94	2,499,311.87	5,083,351.59
Total Uncosted - Quarterly (Federal and Non-Federal)	5,211,000.00	4,844,493.62	4,341,615.74	3,494,505.72	8,062,375.57

Cost Status (Continued)

Project Title: US-China Clean Energy Research Center Advanced Coal Technology Collaboration

DOE Award Number: DE-PI0000017

YEARS 1-7 Start: 10/01/10 End: 09/30/2015

Baseline Reporting Quarter	Q6 (3/31/12)	Q7 (6/30/12)	Q8 (9/30/12)	Q9 (12/31/12)	Q10 (3/31/13)
Baseline Cost Plan	(From 424A, Sec. D)				
(from SF-424A)					
Federal Share				7,500,000	
Non-Federal Share				7,922,000	
Total Planned (Federal and Non-Federal)				15,422,000	
Cumulative Baseline Costs					
Actual Incurred Costs					
Federal Share	393,669.67	899,387.50	406,156.70	498,753.07	440,928.74
Non-Federal Share	671,649.51	554,069.94	887,549.37	382,036.74	1,313,008.54
Total Incurred Costs - Quarterly (Federal and Non-Federal)	1,065,319.18	1,453,457.44	1,293,706.07	880,789.81	1,753,937.28
Cumulative Incurred Costs	3,424,943.61	4,878,401.05	6,172,107.12	7,052,896.93	8,806,834.21
Uncosted					
Federal Share	2,585,354.31	1,685,966.81	1,279,810.11	3,281,057.04	2,840,128.30
Non-Federal Share	4,411,702.08	3,857,632.14	2,970,082.77	5,088,046.03	3,775,037.49
Total Uncosted - Quarterly (Federal and Non-Federal)	6,997,056.39	5,543,598.95	4,249,892.88	8,369,103.07	6,615,165.79

Project Title: US-China Clean Energy Research Center Advanced Coal Technology Collaboration

DOE Award Number: DE-PI0000017

YEARS 1-7 Start: 10/01/10 End: 09/30/2015

Baseline Reporting Quarter	Q11 (6/30/13)	Q12 (9/30/13)	Q13 (12/31/13)	Q14 (3/31/14)	
Baseline Cost Plan	(From 424A, Sec. D)				
(from SF-424A)					
Federal Share			10,000,000		
Non-Federal Share			10,422,000		
Total Planned (Federal and Non-Federal)			20,422,000		
Cumulative Baseline Costs					
Actual Incurred Costs					
Federal Share	1,157,140.72	225,538.99	161,228	458,760.16	
Non-Federal Share	834,266.63	987,612.23	590,907.31	788,934.06	
Total Incurred Costs - Quarterly (Federal and Non-Federal)	1,991,407.35	1,213,151.22	752,135.65	1,247,694.22	
Cumulative Incurred Costs	10,798,241.56	12,011,392.78	12,763,528.43	14,011,222.65	
Uncosted					
Federal Share	1,682,987.58	1,457,448.59	3,796,220.25	3,337,460.09	
Non-Federal Share	2,940,770.86	1,953,158.63	3,862,251.32	3,073,317.26	
Total Uncosted - Quarterly (Federal and Non-Federal)	4,623,758.44	3,410,607.22	7,658,471.57	6,410,777.35	

Appendices:

Appendix I

Theme 6.4.B – Action Plan

Action Plan

Project years 4 and 5

CERC_ACTC Theme 6

Carbon Capture, Utilization, and Storage (CCUS) system modeling of the Ordos basin (China) and Illinois Basin (USA).

Bing Bai, IRSM

John Rupp, IGS

Kevin Ellett, IGS

Philip Stauffer, LANL

Richard Middleton, LANL

January 21, 2014

Background

The Ordos Basin is China's second-largest sedimentary basin in the mid-western region of the country. It boasts widespread resources in its vast area. These many kinds of energy and mineral resources are characterized by huge potential and considerable reserves. It contributes most to the reserves of natural gas, coal bed methane, and coal already proven in China, accounting for nearly 6%, 13%, and 20%, respectively. As a typical cratonic basin, Ordos basin has its special characteristics, such as gentle structure, deep reservoir, overlapped sand and mud, thin bed and sharp lateral variation, etc. Much research shows that it has a potentially large storage capacity and very good conditions for secure CO_2sequestration. Comparatively speaking, Ordos basin has had a high degree of research and exploration, and much geological data or information has been accumulated. All these attributes are very similar to that of the Illinois Basin, USA.

Comparison of geological and surface infrastructure information is necessary to advance CCUS research and its subsequent applications in both basins. Critical to this comparison is the accessibility by researchers on both teams to have access to information that will be used to make the analyses. The U.S. team has already built a suite of datasets that characterize aspects of the Illinois Basin and is prepared to use subsets of these data to demonstrate an analysis workflow with the China team. However, to date, a comparable comprehensive dataset for the Ordos basin, based on Chinese information, has yet to be compiled. On the other hand, significant amounts of research and exploration data have been accumulated for the Ordos basin. Much of these existing data are distributed within private oil & gas company's holdings. But some is available in the public domain, existing in the files of research institutes and within the public literatures.

To meet this need for obtaining mutual access to comparable information, at the Jackson Hole, WY meeting of CERC-ACTC, held in October 2-3 2013, representatives of the American and Chinese research teams proposed to collect, compile and integrate the existing data from China public channels and then build a 3D geological model of Ordos basin based on the approach used for the Illinois basin.

Strategic Goal

The Ordos Basin and the Illinois Basin were chosen respectively as the primary research targets for China and USA teams in CERC-ACTC Theme 6. The goal of this Theme is to develop project-ready, commercial-scale geological CO_2 storage, EOR and ECBM capabilities in China and USA.

Objectives

To accomplish this goal, the teams will investigate and compare, using a variety of methods and differing data types and densities, the CO_2 reservoir capacity and injectivity, seal integrity, utilization potential, and CCUS infrastructure for both basins. Initially, lessons learned from work already completed for the Illinois basin will help develop and validate evaluation methodologies for the Ordos basin. Additionally, as work on the

Ordos progresses, lessons learned in the analysis of the Ordos will provide important feedback for future assessment work in the Illinois basin.
To effectively complete these comparisons, the Chinese team will compile the needed information for the Ordos basin to compare with the information previously compiled by the U.S. team for the Illinois basin.

After creating a geologic model of the Ordos and compiling the data sets for CCUS infrastructure, the CO_2 storage capacity, injectivity, seal integrity, utilization potential, and infrastructure development options will be analyzed. Initially, CCUS options will be investigated using 30 x 30 km parcels of each basin.

The final stage will be the comparison of the interpretations of the two basins using a variety of techniques. The objective of this effort will be to determine the most effective and efficient means to assess storage capacity and utilization scenarios. The results of this comparison will be useful in assessing these capacities in other portions of China and the U.S.

The Chinese Academy of Sciences (CAS) team will work with CERC members Yangchang Oil and the Northwestern University to combine existing public domain data for the Ordos basin. Interaction with Zhou Lifa (XX) along with Jiao Zunsheng and Ron Surdam (UW), will be crucial for interpreting the Chinese information. Additionally, the experience of Yangchang Oil with EOR is an important contribution to the utilization component of CCUS. This work has been included in the work plans of theme 6 for years 4 + 5 on both the U.S. and Chinese sides of the CERC.

Products

- Collect, Compiled, integrated and shared existing public geological and infrastructure datasets
- 3D eological models of both basins
- CO_2 storage capacities and injectivity scenarios for the Ordos and Illinois basins,
- Evaluation of the seal integrity over some of the key storage reservoirs
- Analysis of potential for utilizing CO2 in extraction of hydrocarbons (EOR, ECBM)
- Investigation of possible infrastructure developments for a range of CCUS scenarios
- Publications, presentations and reports of these analyses

Intellectual property and data use

The results of the work mean all technological achievements such as Intellectual Property Rights in the course of the work. Such Intellectual Property Rights which are generated from this work are hereinafter referred to as "Relevant Intellectual Property Rights."

The relevant Intellectual Property Rights belong to all the contributing member institutions who automatically have priority to access the output data and information. A time span will be defined to protect the priority of the contributing members (2 years). When the duration of protection ends (End of CERC), the output can be freely distributed by any of the contributing member institutions. Anyone can access the output data provided that a use protocol is signed.

Work Plan

- Learn lessons from the geological modeling of Illinois Basin.

  As the "kick-off" of the work, we should have an intensive learning from the work of Illinois basin modeling since the American team has already accumulated a lot of experiences. The Chinese team doesn't have much experience on basin scale geological modeling. The initial goal of the project will be to focus on a parcel (30 x 30 km) the Ordos basin to demonstrate the gain in understanding as more data is included in the analysis. This requires finding a site that has a good amount of borehole, seismic, pump-test, and infrastructure data. This small initial model size will allow for a fast turn-around of results and permit the Chinese team to learn more quickly.

  To achieve the target, the American team will share necessary documents or reports of the Illinois basin modeling and assist in algorithm use.

- Iterative development strategy

  Considering the complexity and many uncertainties of this work and the data, it is nearly impossible to reach perfection at one stroke. An iterative development strategy will be adopted to guide the whole work. This will avoid the "semi - finished products" and ensure us produce beneficial outcomes to satisfy the application needs in limited time. Subsequent updating will give better evolution editions.

- Develop a common methodology to assess the storage potential through comparisons of existing methodologies to optimize the analytical techniques and facilitate comparison of results.

  There already exist some storage assessment methodologies. These methodologies may need further developed to reflect the practices and specific conditions. But the updating should be based on the detailed comparison and tests of these existing methodologies using high quality data. It is expected a common optimized methodology accepted by both sides be developed. As methodologies are developed, they will be applied to the Ordos and Illinois basins.

- Sufficient work and preparation for workshop or meeting

  It is not easy for US. and China participants to get together frequently. To make the workshop cost & time effective and efficient, sufficient work and preparation (emails, telephone, internet, etc.) through communications should be made. This includes collaboration with all partners on both the U.S. and Chinese sides of the CERC (CAS, LANL, IGS, Yangchang Oil, UWY, NWU, and CUMT). Of particular importance for the Ordos basin will be the sharing of information among the Chinese CERC partners.

- Frequent minding and push will make the work move forward fast. To this end we recommend daily to weekly interactions between individuals and monthly team meetings as time permits.

Participants and responsibility

No.	Participants	Institution	Responsibility
1	Jun Li	IRSM	*Execution* *Action plan, Management* *Data and literature collection, compilation and integration, modeling*
2	Bing Bai	IRSM	*Specific data collection and compilation*
3	Xiaochun Li	IRSM	*Lead, China funding, guidance, management*
4	Ning Wei	IRSM	*Existing data compilation & submission*
5	Ellett, Kevin Michael	IGS	*Execution,* *Existing data compilation & submission;* *Technical guidance & consultance*
6	John Rupp	IGS	*Lead, US. Funding, guidance, advice, check*
7	Zunsheng Jiao	UW	*Existing data and reference compilation & submission; guidance, advice, check*
8	Philip H. Stauffer	LANL	*Technical guidance & consultance, check*
9	Richard S. Middleton	LANL	*Technical guidance & consultance, check*
10	Ron Surdam	UW	*Ordos Basin, EOR, Characterization Expert*
11	? ?	Yangchang	*EOR and Ordos borehole data*

Data sources and range

As the geological data are massive, initial targets of which data should be prioritized to limit the amount of data processed. Within this initial effort, the purpose of geological modeling of Ordos basin is to support the sub-basin scale CO_2 storage capacity, sealing ability, stability evaluations, source-sink matching & pipeline planning (which needs injectivity etc.) evaluation.

Limited by the proprietary nature of some of the data and/or security acts in China, only the data from the publicly published literature will be collected from Chinese sources for

the evaluation of the Ordos basin. The literature sources include: books, thesis, atlas, maps, journal papers and public reports etc. This will ensure the data exchange and cooperation is effective and open.

Work flow and stages

1. Literature review and compilation of public datasets for Ordos Basin geology (Lead group: CAS) and Illinois Basin geology (Lead Group: IGS)s
2. Development of specific geological targets and approaches for 3D geological modeling (CAS and IGS) and CCUS modeling (Leads: LANL and UWY)
3. Complete templates of the data parameters that are necessary for the modeling approaches defined in setup 2 (CAS and IGS)
4. Conduct workshop on 3D modeling of characteristics of selected geological reservoirs and CCUS (EOR and storage). IGS to lead with Illinois Basin dataset, followed by CAS with Ordos Basin dataset. LANL and UWY to finish with CCUS modeling (CO2 injection simulation for EOR, storage, and pipeline optimization.
5. Research collaboration based on workshop results and publication of findings

Work schedule

No.	Tasks	Time duration	Status	Note
1	Work plan, preparation	Nov.-Dec 2013	ongoing	
2	Comprehensive literature retrieval	Nov.2013 - Jan.,2014	ongoing	
3	Collecting public data reference sources	Dec. 2013- Mar. 2014	ongoing	
4	Discuss and determine the specific targets of the geological modeling and CCUS modeling	Feb. 2014		Based on 3
5	Determine the specific modeling schemes and contents	Feb.- Mar.,2014		
6	Preliminary reference summarizing,compiling:digitizing,vectorizing, skimming, classification	Feb.- March, 2014		
7	Develop the templates of data forms to fill in the necessary modeling parameters	Feb.- March,2014		Based on 5 and 6
8	Complete the targeted data forms.	Mar.- Apr.,2014		
9	Workshop on 3D geological modeling and CCUS modeling by informational exchange on Illinois and Ordos Basins	May,2014		
10	Follow up analysis and publication of findings	Jun.-Dec., 2014		

Appendix I

Theme 6.4.B – Theme 6 Workshop on Geological Modeling, its potential applications in Ordos and Illinois Basins

Agenda (May 4-9, 2014, IRSM,Wuhan, Hubei, China)Sunday May 4th 2014

Time	Presentation Title	By	From	Notes
8:30-8:40	Welcome	Xiaochun Li	IRSM	
	Group picture	All	All	
8:40-9:00	Pls fill	John A. Rupp	IGS	
9:00-9:20	Pls fill	Philip Stauffer	LANL	
9:20-9:40	Pls fill	Zunsheng Jiao	UW	
9:40-10:00	Pls fill	Jeff Wagoner	LLNL	
10:00-10:20	Pls fill	Sarah Forbes	WRI	
10:20-10:30	Tea Break			
10:30-10:50	Pls fill	Lifa Zhou	SPIERCE	
10:50-11:10	Pls fill	?	Yanchang Group	
11:10-11:30	Pls fill	Ruina Xu ?	Tsinghua	
11:30-11:50	Pls fill	Ruizhao Yang	CUMTB	
11:50-12:00	Short summary	All	All	
12:00-13:00	Lunch (Oak Fruit Rest.)			
13:00-14:30	Noon rest(Hotel)			
14:30-14:50	Pls fill	Shaoliang Zhang	CUMT	
14:50-15:10	Pls fill	Xiaochun Li	IRSM	
15:10-15:20	Select drafters for by-lateral discussion			
15:20-15:40	Define outcomes for Theme 6 year 5 （Phil please prepare a draft）	Philip Stauffer & Xiaochun Li	US&China	John A. Rupp hosts
15:40-16:10	CERC2.0 message exchange	US: ? China：Xiaochun Li	US&China	
16:10-16:20	Short break			
16:20-16:50	Define outcomes for workshop and Agenda confirmation(Bing Bai prepares a draft)	All	All	John A. Rupp hosts
16:50-17:10	Short summary	All	All	
18:00	Dinner	Jinsanli		

Monday May 5th 2014

Time	Presentation Title	By	From	Notes
9:00-9:05	Open	Xiaochun Li		
9:05-10:05	Details of Illinois Basin geological model construction using Petrel and ArcGIS.	Kevin M. Ellett	IGS	
10:05-10:25	Questions			
10:25-10:35	Short break			
10:35-11:35	Details of Illinois Basin integrated system modeling for source-sink matching using SimCCS and CO2-PENS.	Philip Stauffer, Richard S. Middleton	LANL	
11:35-11:45	Questions			
11:45-12:00	Morning Summary	All	All	Xiaochun Li Holds
12:00-13:00	Lunch (Oak Fruit Rest.)			
13:00-14:30	Noon rest(Hotel)			
14:30-15:45	Progress on Ordos Basin geological model construction	Li Jun	IRSM	
15:45-16:15	Questions	All	All	
16:15-17:00	Other data source discussions	Li fa zhou, Zunsheng Jiao, Ning Wei, CUMT		
17:00-17:30	Data sharing method			
18:00	Dinner	Jinsanli		

Tuesday May 6th 2014

Time	Presentation Title	By	From	Notes
9:00-9:05	Open	Xiaochun Li		
9:05-10:05	Details of EOR studies and basin-wide EOR potential resources	Jiao Zunsheng, Zhou Lifa	UW,SPI ERCE	
10:05-10:25	Questions			
10:25-10:35	Short break			
10:35-11:00	Feasibility study on Guohua plant Oxfuel combustion-aquifer storage	Ning Wei, Zunsheng Jiao	IRSM	
11:00-11:25	Questions			
11:25-11:40	Potential applications of Geological model : capacity evaluation review and ideas	Bing Bai, John A. Rupp	IRSM, IGS	
11:40-11:50	Questions			
11:50-12:00	Summary			
12:00-13:00	Lunch (Oak Fruit Rest.)			
13:00-14:30	Noon rest(Hotel)			
14:30-17:45	Face to face discussions on specific technical issues,free activities			
18:00	Dinner	Jinsanli		

Wednesday May 7th 2014

Time	Action	Where	Notes
Befor 7:00	Wait	at the 1st floor of the hotel	BaiBing accompanies
7:00	Depart	to the Train Station	
7:30-9:30	On the way	to Yichang city	Two hours
10:00-17:30	Sightseeing	at Three Gorges	
17:30-19:00	Dinner	near the Yichang station	
19:40-21:41	Return back	to Wuhan	Two hours

Thursday May 8th 2014

Time	Presentation Title	By	From	Notes
9:00-9:05	Open	Li Xiaochun	IRSM	
9:05-9:55	Specific plan on next step Geological model construction (Li Jun please prepare a draft for discussion)	Li Jun	All	Li Xiaochun hosts
9:55-10:10	Short break			
10:10-11:00	Data sharing Strategy, principles (Bing Bai please prepare a draft for discussion)	Bing Bai	IRSM	
11:00-11:40	Potential applications of of geological models and future outputs, deliverable	Philip Stauffer	LANL	John
11:40-12:00	Summary	All	All	
12:00-13:00	Lunch (Oak Fruit Rest.)			
13:00-14:30	Noon rest(Hotel)			
14:30-17:45	Face to face discussion			
18:00	Dinner	Jinsanli		

Friday May 9th 2014

Time	Presentation Title	By	From	Notes
9:00-9:05	Open	Li Xiaochun	IRSM	
9:05-10:05	Workshop products finalized and Resolution discussion(Please prepare workshop products and the ACTC2.0 IDEAS drafts)	Drafters		John hosts
10:05-10:25	Break			
10:25-11:25	Schedule tasks to meet Year 4 product goals	All		Phil hosts
11:25-12:00	Summary and close	All	All	
12:00-13:00	Lunch (Oak Fruit Rest.) and Bye Bye			
	To the airport			

Participants

No.	Participants	Institution	reservations	Room type	Status
1	John A. Rupp	IGS	check in on May 3 and check out on May 9th	single room	**Reserved**
2	Kevin M. Ellett	IGS	check in on May 3 and check out on May 9th	single room	**Reserved**
3	Zunsheng Jiao	UW	5 月 2 日—5 月 9 日	single room	**Reserved**
4	Philip Stauffer	LANL	checking in late on Friday May 2nd and Checking out early on Saturday May 10	single room	**Reserved**
5	Richard S. Middleton	LANL	Erin and I will check in on Friday May 2nd and check out on Friday May 9th.	Double Room	**Reserved**
6	Jeff Wagoner	LLNL	check in on May 2 and check out on May 9th	single room	**Reserved**
7	Xiaoliang Yang	WRI	5 月 2 日—5 月 9 日	single room	**Reserved**
8	Lifa Zhou	SPIERCE	5 月 2 日—5 月 9 日	single room	**Reserved**
9	Sarah Forbes	WRI	5 月 2 日—5 月 9 日	single room	**Reserved**