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Final Report

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Abstract

The overall objective of the project is to demonstrate the technical and economic viability of a new Integrated Gasification Combined Cycle (IGCC) power plant designed to efficiently process low rank coals. The plant uses an integrated CO₂ scrubber/Water Gas Shift (WGS) catalyst to capture over 90 percent of the CO₂ emissions, while providing a significantly lower cost of electricity (COE) than a similar plant with conventional cold gas cleanup system based on Selexol™ technology and 90 percent carbon capture. TDA's system uses a high temperature physical adsorbent capable of removing CO₂ above the dew point of the synthesis gas and a commercial WGS catalyst that can effectively convert CO in bituminous coal. The overall objective of the project is to demonstrate the technical and economic viability of a new Integrated Gasification Combined Cycle (IGCC) power plant designed to efficiently process low rank coals. The plant uses an integrated CO₂ scrubber/Water Gas Shift (WGS) catalyst to capture over 90 percent of the CO₂ emissions, while providing a significantly lower cost of electricity (COE) than a similar plant with conventional cold gas cleanup system based on Selexol™ technology and 90 percent carbon capture. TDA's system uses a high temperature physical adsorbent capable of removing CO₂ above the dew point of the synthesis gas and a commercial WGS catalyst that can effectively convert CO in bituminous coal. The net plant efficiency is about 2.4 percentage points higher than an Integrated Gasification Combined Cycle (IGCC) plant equipped with Selexol™ to capture CO₂. We also previously completed two successful field demonstrations: one at the National Carbon Capture Center (Southern- Wilsonville, AL) in 2011, and a second demonstration in fall of 2012 at the Wabash River IGCC plant (Terra Haute, IN). In this project, we first optimized the sorbent to catalyst ratio used in the combined WGS and CO₂ capture process and confirmed the technical feasibility in bench-scale experiments. In these tests, we did not observe any CO breakthrough both during adsorption and desorption steps indicating that there is complete conversion of CO to CO₂ and H₂. The overall CO conversions above 90 percent were observed. The sorbent achieved a total CO₂ loading of 7.82 percent wt. of which 5.68 percent is from conversion of CO into CO₂. The results of the system analysis suggest that the TDA combined shift and high temperature PSA-based Warm Gas Clean-up technology can make a substantial improvement in the IGCC plant thermal performance for a plant designed to achieve near zero emissions (including greater than 90 percent carbon capture). The capital expenses are also expected to be lower than those of Selexol. The higher net plant efficiency and lower capital and operating costs result in substantial reduction in the COE for the IGCC plant equipped with the TDA combined shift and high temperature PSA-based carbon capture system.

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Executive Summary

The overall objective of the project is to demonstrate the technical and economic viability of a new Integrated Gasification Combined Cycle (IGCC) power plant designed to efficiently process low rank coals. The plant uses an integrated CO₂ scrubber/Water Gas Shift (WGS) catalyst to capture over 90% capture of the CO₂ emissions, while providing a significantly lower cost of electricity (COE) than a similar plant with conventional cold gas cleanup system based on Selexol™ technology and 90% carbon capture.

TDA's system uses a high temperature physical adsorbent capable of removing CO₂ above the dew point of the synthesis gas and a commercial WGS catalyst that can effectively convert CO in the synthesis gas generated from gasification of low rank coals into H₂ and CO₂. The integrated operation of the WGS catalyst and CO₂ removal processes in a single step drives the equilibrium-limited WGS reaction towards hydrogen without the need to add large amounts of water to the synthesis gas, greatly reducing the cost of carbon capture. In a previous DOE/NETL sponsored project, TDA has already developed the sorbent for pre-combustion CO₂ capture (Contract No. DE-FE0000469) and successfully scaled-up the production of the new sorbent. We demonstrated stable CO₂ capacity for over 12,650 cycles at the bench-scale. A process analysis carried out by University of California, Irvine showed that for bituminous coal the net plant efficiency is about 2.4% points higher than an Integrated Gasification Combined Cycle (IGCC) plant equipped with Selexol to capture CO₂. We also previously completed two successful field demonstrations: one at the National Carbon Capture Center (Southern-Wilsonville, AL) in 2011, and a second demonstration in fall of 2012 at the Wabash River IGCC plant (Terra Haute, IN).

In this project, we first optimized the sorbent to catalyst ratio used in the combined WGS and CO₂ capture process and confirmed the technical feasibility in bench-scale experiments. In these tests, we did not observe any CO breakthrough both during adsorption and desorption steps indicating that there is complete conversion of CO to CO₂ and H₂ (Figure 1).

The overall CO conversions

above 90% were observed. The sorbent achieved a total CO₂ loading of 7.82% wt. of which 5.68% is from conversion of CO into CO₂.

Figure 1. Combined WGS/CO₂ capture with 10% (vol.) Shiftmax 230 in TDA's CO₂ sorbent – AMS-19. CO in the feed and product.

In a laboratory-scale reactor, we have demonstrated the cyclic activity of the combined WGS and CO₂ capture process and life of the material for over 1,140 adsorption/regeneration cycles under representative conditions. In these cycles, the sorbent and the catalyst maintained their CO₂ adsorption capacity and CO conversion without any signs of degradation (Figure 2). Extensive characterization of the sorbent following the multiple cycle tests suggests that the

physical and chemical characteristics of the sorbent (e.g., surface area, active material content) remained intact.

Based on the bench-scale test results, TDA designed a pressure swing adsorption (PSA) cycle sequence for the combined WGS and CO₂ capture process that consists of 8 beds with multiple steps such as adsorption, depressurization, pressure equalization, desorption and steam purge, etc. all of which ensures continuous removal of CO₂ from the synthesis gas. The system generates a concentrated CO₂ stream ready for further purification

and compression and also a very low CO₂ containing synthesis gas fuel to be burned in the gas turbine. The PSA cycle sequence was optimized using a Fortran code developed by University of Michigan. Based on the simulation results, TDA completed the design of the CO₂ separation, purification and compression process. For a nominal 600 MW IGCC plant, the CO₂ removal system consists of three trains of 8-bed PSA units; total of 24 beds housing the sorbent.

Figure 2. CO₂ capacity of the sorbent in multiple pressure swing cycles tests in a split bed configuration.

Figure 3. TDA's field demonstration unit; (a) the 4-bed high temperature PSA-based CO₂ separation sub-assembly; (b) synthesis gas conditioning sub-assembly, (c) TDA's field demonstration unit installed at the Power Systems Demonstration Facility.

In collaboration with the Southern Company, TDA carried out slipstream field tests to assess the efficacy of the combined WGS and CO₂ capture process from actual coal-derived synthesis gas. We modified a fully automated test unit that has 4 high temperature PSA beds to house the catalyst-sorbent mixture (although the slipstream test unit did not use the 8-bed configuration selected for the final design, the selected configuration was more than adequate for

demonstrating all critical aspects of the concept within the budget and schedule constraints of this project). The field test unit also included an additional synthesis gas conditioning sub-assembly, with options for bulk sulfur removal, steam injection and water-gas-shift synthesis to adjust the synthesis gas concentration and purity. Figure 3 shows the pictures of the field demonstration unit, including the CO₂ separation and synthesis gas conditioning sub-assemblies. This unit was previously built under a DOE/NETL funded project (Contract# DE-FE-0000469) and modified and upgraded to carry out the tests on this project.

Figure 4. Carbon capture rates during a portion of testing.

In these field tests, the CO conversion at a steam:CO ratio of 1.1 is 96.4% compared to 91% predicted by the WGS reaction equilibrium at a temperature of 230°C and 200 psig (i.e., over 5% points more than equilibrium conversion). This shift in equilibrium is most likely due to the closely coupled removal of the product gas, CO₂ which enables the reaction to reach closer to completion. The capacity of the sorbent is slightly higher than it was in the last campaign (carried out under DE-FE-0000469) due to the decrease in H₂O in the feed stream which raises the CO₂ partial pressure. The field test unit was online for over 600 hours during which approximately 32,000 SCF of coal derived syngas was processed. Figure 4 shows the amount of total carbon entering the prototype unit as CO and CO₂ and the amount of carbon exiting the apparatus along with the high pressure syngas. The average overall carbon capture rate for this demonstration test campaign was over 96%, with an average overall CO conversion of 96.4% at an average steam:CO ratio of 1.1.

An important observation during these tests was that the bed temperature was higher when the catalyst and sorbent operated together compared to previous test campaigns with only the CO₂ sorbent. The heat effects will be more pronounced with higher CO/CO₂ content synthesis gas (as mentioned the NCCC gas was diluted with nitrogen due to the air blown transport gasifier used for gasification of the coal). Hence, there is a need to carry out detailed CFD modeling of the reactor design and the heat management in the PSA beds, which are scheduled as part of a new DOE funded project (DE-FE-0012048).

In collaboration with Phillips 66, and the Advanced Power and Energy Program of the University of California, Irvine (UCI), TDA developed system simulation models using Aspen PlusTM simulation software to assess the economic viability of TDA's combined WGS with high temperature PSA-based pre-combustion carbon capture technology. Phillips 66 provided the performance results for the E-GasTM gasifier operating on two different types of low rank coals:

sub-bituminous and lignite. This included the block flow diagrams and the stream summary report around the gasification system. These results along with the performance results and stream summary around TDA's combined WGS and CO₂ capture unit were integrated into the Aspen Model developed for the cold gas capture system using Selexol and warm gas capture system using TDA's combined shift and PSA-based CO₂ capture system by UCI and detailed system and process economic analysis was carried out. This analysis provided a thorough comparison against a conventional cold gas cleanup technology based on the Selexol™ physical solvent scrubbing for the low rank coals.

The Warm Gas Cleanup system using TDA's combined shift and high temperature PSA-based CO₂ capture system achieved net plant efficiencies of 32.90% and 30.42% (on a coal HHV basis) for the subbituminous and the lignite coals. These net plant efficiencies at 90% carbon capture are significantly higher than those achieved for the corresponding Cold Gas Cases using Selexol™ scrubber at 31.35% and 28.28% (on a coal HHV basis for the subbituminous and the lignite coals respectively) which correspond to about 5% and 7% decrease in the heat rate respectively for TDA's Warm Gas Cleanup system.

The capital expense for the plants were estimated following the "Cost Guidelines provide by DOE/NETL (2007) (e.g. higher contingencies were applied for unproven technologies such as the combined shift and high temperature PSA unit). The plant cost for TDA's Warm gas Cleanup Process is estimated as \$2824/kW and \$2990/kW for the subbituminous and the lignite coals, which are about 6% and 11% lower than those of the corresponding Cold Gas Cleanup Cases at \$2993/kW and \$3348/kW (for the subbituminous and the lignite coals respectively). The levelized cost of electricity including the transport, storage and monitoring (TS&M) costs for CO₂ is calculated as \$100.1/MWh and \$105.8/MWh for the subbituminous and the lignite coal cases with TDA's Warm gas Cleanup technology. The corresponding costs for the Cold Gas Cases using the Selexol™ scrubbing technology are calculated as \$105.3/MWh and \$117.0/MWh (for the subbituminous and the lignite coals respectively).

Table 1. Comparison of TDA's Warm Gas Cleanup against Selexol™ based Cold Gas Cleanup System with fully loaded GE F class type gas turbines.

Coal Type	Subbituminous		Lignite	
	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent
Raw Gas Cleanup Option				
CO ₂ Capture, %	90	90	90	90
Gross Power Generated, kWe	692,955	685,211	746,456	756,407
Gas Turbine Power	430,900	430,900	456,600	456,600
Steam Turbine Power	262,055	254,311	289,856	299,807
Auxiliary Load, kWe	181,112	134,862	241,194	158,416
Net Power, kWe	511,843	550,349	505,262	597,992
Net Plant Efficiency, % HHV	31.35	32.90	28.28	30.42
Coal Feed Rate, kg/h	295,046	302,251	417,873	459,799
Raw Water Usage, GPM/MWe	7.4	7.7	9.0	9.3
Total Plant Cost, \$/kWe	2,993	2,824	3,348	2,990
COE without CO ₂ TS&M, \$/MWh	99.5	94.6	110.4	99.8
COE with CO ₂ TS&M, \$MWH	105.3	100.1	117.0	105.8

The results of the system analysis suggest that TDA's combined shift and high temperature PSA-based Warm Gas Clean-up technology can make a substantial improvement in the IGCC plant thermal performance for a plant designed to achieve near zero emissions (including greater than 90% carbon capture). The capital expenses are also expected to be lower than those of Selexol's™. The higher net plant efficiency and lower capital and operating costs result in substantial reduction in the COE for the IGCC plant equipped with TDA's combined shift and high temperature PSA-based carbon capture system.

1. Introduction

Coal accounts for 56% of U.S. power generation and its contribution is expected to increase since U.S. has 25% of world's coal reserves (Tonks 2007). Coal-fueled IGCCs are environmentally superior to pulverized coal (PC)-fired boilers not only because they are more efficient at producing electricity, but also they can be equipped with more cost effective carbon capture and pollution control technologies. Since half of the coal in the U.S. is low rank (e.g., high in alkali and moisture), it is expected that most of the new IGCC installations will use these feedstocks. Unfortunately, the system analysis carried out by DOE (DOE/NETL-2007/1281) suggests that conventional low temperature technologies used to capture CO₂ from an IGCC (such as Selexol) will increase the COE to prohibitive levels. Hence, new technologies are needed to meet DOE's goal of capturing 90% of the carbon with less than 10% increase in the COE.

TDA Research has developed a new carbon capture technology that can be used in IGCC plants that run on low rank coals. A critical component of the proposed system is an integrated WGS catalyst/high temperature CO₂ scrubber. Figure 5 shows a simplified schematic of our technology integrated with an IGCC plant based CoP's E-Gas™ Gasifier (we used the E-Gas™ system as an example, the proposed technology will work with any gasifier type). As in Wabash River IGCC plant, following the gasifier, the synthesis gas passes through a high temperature heat recovery system that generates high quality steam for the steam cycle. The particulate removal is carried out with high temperature filters, where the char is recycled back to the gasifier.

Figure 5. TDA's CO₂ capture system integrated with CoP's E-Gas™ gasifier.

The particulate-free gas then feeds a water scrubber that operates at 371°C; water scrubbing effectively removes halides, ammonia and some of the trace metals, as well as the water-soluble Na and K compounds (e.g., NaCl, KCl). The high gas temperature prior to the scrubber will prevent the condensation of alkali compounds in the process equipment upstream of the scrubber (as suggested by literature and TDA experiments). The equipment downstream of the scrubber is also protected as the alkali concentration of the gas will be significantly reduced. The relatively low temperature ensures high solubility and capture of contaminants, and limits the amount of water introduced to the synthesis gas.

Following the water scrubber, the syngas will be desulfurized using a regenerable zinc oxide based sorbent (similar to RVS-1 or Z-Sorb developed by RTI and CoP, respectively). After the desulfurizer, the gas passes through a stand-alone WGS catalyst bed, using a commercial WGS catalyst such as Sud-chemie's Sour Shift catalyst or Shiftmax-120, a Cu/Zn based low temperature shift catalyst or TDA's contaminant tolerant Pt/CeO₂ catalyst. The WGS catalyst bed will effectively convert CO, H₂O into H₂, CO₂. In previous CO₂ adsorption/ carbon capture systems developed by TDA, the shifted synthesis gas is then sent to TDA's CO₂ capture unit at temperatures above the dew point of the synthesis gas for CO₂ removal.

CO₂ capture systems in a physical adsorbent loaded into fixed bed reactors. Sorbent regeneration is carried out by a combination of pressure swing and concentration swing. CO₂ is adsorbed at high pressure (500 to 900 psia depending on the gasifier type) and then the sorbent is regenerated in a two-stage process (Figure 6). First, the bed pressure is reduced to 150 psia to recover the bulk of the CO₂ in a concentrated, pressurized form (which is further compressed to 2,200 psia sequestration pressure). The pressure swing is followed by a steam sweep; the low pressure sweep minimizes the steam use and hence the amount of steam that must be extracted from the steam cycle. In this second stage, the chemical potential for transferring CO₂ from the adsorption side (synthesis gas) to the regeneration side (steam) is provided by the CO₂ partial pressure difference, and there is sufficient driving force at both ends of the process. The outlet gas from regenerator contains CO₂ and steam. Steam is condensed and the CO₂ is purified and pressurized for transport and sequestration. TDA's sorbent achieves a high CO₂ capacity and removal efficiency greater than 90% at temperatures well above the dew point of all commercial gasifiers, including GE water quench gasifier. This eliminates the condensation of the steam in the synthesis gas and maximizes the mass flow through the gas turbine, thereby increasing efficiency of the power cycle.

Figure 6. The CO₂ partial pressure swing that drives the TDA process.

In this project, we worked on combining the two unit operations WGS and CO₂ removal into a single process unit; the process intensification will not only reduce the capital cost by eliminating several reactors, but also increase the WGS conversion at low steam:carbon ratios, leading to further efficiency improvements. In conventional systems, large amounts of water are introduced to the gas to shift the equilibrium and achieve high CO conversion (since carbon capture technologies only remove CO₂ but not CO, it is critical to shift as much CO as possible). In addition to using an excess of water, the conventional systems also achieve high CO conversion through effective thermal management. For example, 3-stage reactor systems with inter-stage cooling are used to maintain a low gas temperature to ensure high CO conversion (since WGS is exothermic, higher equilibrium conversions can be achieved at low temperature). However, the use of multiple reactor and heat exchangers increases process cost. The proposed *in situ* removal of CO₂ during the WGS process will drive the equilibrium-limited WGS reaction to completion and increases the H₂ yield at low steam partial pressures.

The combined WGS/CO₂ capture block consists of a WGS/CO₂ separation system (the high temperature PSA system, which uses a mixed bed of WGS catalyst and TDA's CO₂ sorbent) and a purification/compression system, which further treats the CO₂ stream from the separation unit into a pure, pressurized CO₂ product that meets pipeline specification. TDA's high temperature PSA-based WGS/CO₂ separation system converts the residual CO into CO₂ (achieving overall CO conversions as high as 98+% with an average of 96.4%) while capturing 90% of the carbon from the synthesis gas as CO₂ and produces a CO₂-lean synthesis gas (primarily H₂ and H₂O) that is sent to the gas turbine. Any gases trapped in the voids of the sorbent and the reactor ullage space are recovered at an intermediate pressure and recycled back to the synthesis gas feed to ensure high H₂ recovery in the CO₂ separation unit. A steam purge at lower pressure is used to fully regenerate the sorbent.

A CO₂ rich stream primarily consisting of H₂O and CO₂ (along with some CO and H₂ impurities) is sent for further purification and compression to produce high purity CO₂ at 2,200 psig that can be sent for sequestration. For CO₂ purification a catalytic combustor is used to burn any residual syngas with oxygen. In this approach pure oxygen is used to oxidize any H₂, CO and CH₄ remaining in the concentrated CO₂ stream, converting them into CO₂ and H₂O. After dehydration, CO₂ was pressurized. The catalytic combustion of impurities provided a CO₂ product purity comparable to that can be achieved by SelexolTM.

2. Project Objectives

The overall objective of the project is to demonstrate the technical and economic viability of a new Integrated Gasification Combined Cycle (IGCC) power plant designed to efficiently process low rank coals. The plant uses an integrated CO₂ scrubber/Water Gas Shift (WGS) catalyst to capture over 90% capture of the CO₂ emissions, while providing significantly lower cost of electricity (COE) than a similar plant with conventional cold gas cleanup system based on Selexol™ technology with 90% carbon capture.

TDA's system uses a high temperature physical adsorbent capable of removing CO₂ above the dew point of the synthesis gas and a commercial WGS catalyst that can effectively convert CO in the synthesis gas generated from gasification of low rank coals into H₂ and CO₂. The integrated operation of the WGS catalyst and CO₂ removal processes in a single step drives the equilibrium-limited WGS reaction towards hydrogen without the need to add large amounts of water to the synthesis gas, greatly reducing the cost of carbon capture. Our preliminary system analysis suggest that maintaining the H₂O:C ratio close to that required by the reaction stoichiometry rather than using an excess of close to 2.0 (which was the basis of a recent DOE analysis) will improve process efficiency by more than 2%. In addition process intensification provided by carrying out two unit operations (WGS and CO₂ removal) in the same reactor will further reduce the capital cost and improve the process economics.

In a previous DOE/NETL sponsored project, TDA has already developed the sorbent for pre-combustion CO₂ capture (Contract No. DE-FE0000469) and successfully scaled-up the production of the new sorbent. We demonstrated stable CO₂ capacity for over 12,650 cycles at the bench-scale. A process analysis carried out by University of California, Irvine showed that for bituminous coal the net plant efficiency is about 2.4% points higher than an Integrated Gasification Combined Cycle (IGCC) plant equipped with Selexol to capture CO₂. We also successfully completed two field demonstrations: one at the National Carbon Capture Center (Southern- Wilsonville, AL) in 2011, and a second demonstration in fall of 2012 at the Wabash River IGCC plant (Terra Haute, IN).

In this project TDA worked with UCI, Southern Company and ConocoPhillips to demonstrate the viability of the new technology (combined WGS and CO₂ capture above dew point of synthesis gas). We will optimize the sorbent/catalyst and process design, and assess the efficacy of the integrated WGS/CO₂ capture system, first in bench-scale experiments and then in a slipstream field demonstration using actual coal-derived synthesis gas (to date our sorbent and catalyst have only been tested separately). Our results will feed into a techno-economic analysis using Aspen Plus™ software to estimate the impact of the contaminant tolerant WGS catalyst/CO₂ capture system on the thermal efficiency of the plant and COE. All analyses will be consistent with DOE/NETL Cost Estimation Guidelines.

We will partner with Southern Company to carry out a 3 week field test at the National Carbon Capture Center (NCCC), using 100 SCFH synthesis gas slipstream generated in their air-blown pilot-scale gasifier in Wilsonville, AL. Southern Company has long had an interest in using low rank, high sodium lignites as the feedstock for their advanced plant designs. Hence, we will use North Dakota Beulah-Zap lignite in the demonstration work. We will also work with UCI on the process design and optimization. We will calculate mass and energy balances for a commercial scale IGCC plant integrated with our WGS catalyst/CO₂ sorbent technology using Aspen Plus™. UCI will benchmark the performance of the new system against a plant that uses a Selexol-based gas clean-up and carbon capture technology. The analysis will be extended to include

Montana Rosebud sub-bituminous coal as well as North Dakota lignite. TDA will also work closely with ConocoPhillips (a leading developer of gasification systems) who will help us to assess the commercial viability of the new technology, and with MeadWestvaco and SudChemie to address any scale-up and mass manufacturing issues related with the production of the WGS catalyst/CO₂ sorbent combination. All analyses will be consistent with DOE/NETL's Cost Estimation Guidelines).

2.1 Work Plan

In the first six months of this 2 year project we will optimize an effective cost sorbent/catalyst, and evaluate its performance. We will also develop an Aspen-Plus™ model of the proposed system integrated to a baseline IGCC plant and estimate the thermal efficiency of the plant. We will then modify an existing field test unit and demonstrate the key aspects of the process using coal-derived synthesis gas with Southern Company. We will complete the system analysis using DOE analysis guidelines. CoP will work with us to review the results and provide engineering consulting throughout the project. The expected result of this project is the demonstration of a new CO₂ capture system that can be efficiently added to IGCC power plants running on low rank coals.

TDA along with its partners UCI, CoP and Southern will undertake the following 7 tasks: In Task 1 we will carry out all the project management tasks as per the Project Management Plan (PMP). We will provide quarterly progress reports and project spending updates. In Task 2, we will explore the options of integrating the sorbent and catalyst. In Task 3, we will measure the CO₂ adsorption, WGS conversion and record the CO₂ loading as a function of time. We plan to carry out a minimum of 1,000 cycles in a relevant environment to assess the catalyst and sorbent life and compare the physical properties to those of the fresh material. In Task 4, TDA, UCI and CoP will conduct process design and simulations using Aspen-Plus™ software. We will compare the overall process efficiency for the baseline case (IGCC with low temperature CO₂ capture system such as Selexol) with TDA's combined WGS catalyst/CO₂ removal system. In Task 5, UCI will carry out a sensitivity analysis to identify the impact of key operating parameters on process efficiency. A preliminary technology feasibility study will be completed. DOE Guidelines for Carbon Capture and Sequestration (NETL 2005) will be used and cost-adjusted to January 2007 dollars. TDA and UCI will estimate the cost of the system, and the COE for integrated system using specific input for the two different coals listed in the FOA (Montana Rosebud and North Dakota Beulah-Zap coals). CoP will evaluate the commercial viability of the process in comparison to the conventional systems (e.g. Selexol for CO₂ capture and commercial sour shift catalyst for WGS). In Task 6, TDA will modify the prototype test unit that was fabricated for an existing DOE contract (# DE-FE0000469) so that both the CO₂ removal and WGS can be carried out in the same unit. In Task 7, we will carry out field demonstrations at NCCC. After the tests, results will be reviewed and the techno-economic analysis will be completed.

3. Results

3.1 Task 1. Project Management and Planning

The project commenced on October 1, 2011 and updated the PMP based on inputs from the DOE project manager and submitted it to DOE (Milestone# 1-1) on October 7, 2011. The Principal Investigator attended a kick-off meeting held at NETL's facility in Pittsburgh, PA on December 2, 2011 (Milestone# 1-2). A project outline, including company overview and project approach, was presented to the DOE technical staff and other interested parties, including other research groups within the overall project scope. In the second quarter of FY 2012, we participated in the DOE peer review program conducted by ASME. Based on the input from the peer review, we extended Task 2 and 3 by 3-months. So as to do a more thorough optimization of the sorbent/catalyst and the number of shift stages to be combined with the CO₂ removal since heat management becomes a bigger issue as we increase the number of stages that are combined with the CO₂ removal. We completed the sorbent/catalyst optimization task (Milestone#1-3) on May 31, 2012. We also completed modifications to the prototype test system on May 31, 2012 to carry out the combined WGS and CO₂ removal (Milestone# 1-7). We started the multiple cycle tests with the combined WGS and CO₂ sorbent bed and completed over 200 cycles (Milestone# 1-5) on June 29, 2012. Overall, we completed over 1,140 cycles in the multiple cycle tests on December 27, 2012 and the catalyst/sorbent combination achieved a stable CO conversion and working capacity for CO₂. (Milestone# 1-8). The characterization of the tested sample from Task 2 and Task 3, the multiple cycle tests were completed on March 31, 2013 (Milestone #1-4).

There were multiple delays in scheduling the field demonstrations due to gasifier shutdown at NCCC and the back-log that generated. We finally commenced the field test campaign using real coal derived synthesis gas at NCCC in March 2013 and TDA's combined WGS and CO₂ capture was demonstrated in that test campaign for more than 600 hours processing more than 1500 lbs of raw coal derived un-shifted synthesis gas capturing more than 96% of the carbon with an average CO conversion of 96.4% at an average steam:CO ratio of 1.1 (Milestone# 1-10 – April 21, 2013). We completed the Task 4 – Process design and modeling of the baseline IGCC plant on Aspen Plus® for Powder River Basin Subbituminous coal and North Dakota Lignite Coal using Selexol™ for acid gas removal including CO₂ and the advanced case using TDA's combined WGS and CO₂ removal system with warm gas cleanup on June 28, 2013 (Milestone# 1-6). We completed the Task 5: System and process economic analysis and calculated the COE for IGCC plant using low rank coals with cold and warm gas CO₂ capture on August 31, 2013 (Milestone# 1-9). We held a final review meeting with the DOE program and project manager at NETL on December 17, 2013 (Milestone# 1-11).

The project Milestone log is summarized in Table 2.

Table 2. Project Milestone log.

Mile-stone #	Budget Period	Task/ Subtask No.	Milestone Description	Planned Comple-tion	Actual Comple-tion	Verification Method
			Project Start Date	10/1/2011		
1-1	1	1.1	Updated Project Management Plan (PMP)	11/1/2011	10/7/2011	PMP file & Feasibility Report
1-2	1	1.1	Year 1: Kickoff Meeting at NETL (Milestone review meeting)	12/1/2011	12/2/2011	Presentation file
1-3	1	2	Complete Sorbent/Catalyst Optimization	5/31/2012	5/31/2012	Results update
1-4	1	2	Complete Characterization of Tested Samples	3/31/2013	3/31/2013	Results update
1-5	1	3	Complete 200 cycles in the Multiple Cycle Tests	6/30/2012	6/29/2012	Results update
1-6	1	4	Complete Process Design and Modeling	6/30/2013	6/28/2013	Presentation file
1-7	1	6	Complete Modifications to Prototype Test Unit	5/31/2012	5/31/2012	Results update
1-8	1	3	Complete 1,000 cycles in the Multiple Cycle Tests	12/31/2012	12/27/2012	Results update
1-9	1	5	Complete System And Process Economic Analysis	8/31/2013	8/31/2013	Results update
1-10	1	7	Complete Field Tests	9/30/2013	4/21/2013	Results update
1-11	1	1	Final Review Meeting- NETL & Final Report	12/30/2013	12/17/2013	Presentation file & Final Report

3.2 Task 2. Sorbent/Catalyst Optimization

In this task, we carried out bench-scale test in the laboratory using simulated synthesis gas mixture to explore the options of integrating the sorbent and catalyst such as the intimate physical mixing of the sorbent and catalyst pellets, layered beds of catalyst and sorbent or a combination of both layered beds and physical mixture. We identified the critical design parameters including the reaction and adsorption/desorption kinetics, sorbent capacity and CO₂ breakthrough profile, CO conversion, Steam: CO ratio and mass transfer limitations to select the best sorbent-to-catalyst ratio and distribution profile within the reactor.

3.2.1 Bench-scale System Description

We used an automated test apparatus that belongs to Air Products, which is capable of operation at pressures up to 900 psig and temperatures up to 300°C to evaluate the sorbent's performance under representative conditions (Figure 5). The apparatus was built at TDA for the specific purpose of measuring activity of sorbents and catalysts (with minimal dead volume in the reactor ullage space and in the manifolds) for carrying out testing of Air Products high temperature CO₂ sorbents. We modified the apparatus to evaluate the combined WGS catalyst and CO₂ sorbent's performance under representative conditions (Figure 7). In this system, the desired gas mixtures were directed into a fixed-bed micro-reactor that houses granules or pellets of the sorbent. All gas flows are controlled with electronic mass flow controllers. A Waters pump is used to introduce water. After mixing in a manifold, the feed

Figure 7. Air Product's bench-scale sorbent test apparatus for high temperature CO₂ sorbents.

synthesis gas mixture is then directed into the reactor. A valve system allows the gases to bypass the reactor and flow directly to the analytical system for accurate measurement of the feed gas composition.

In typical tests, the sorbent reactor is loaded with 100 mL of 6-30 mesh size catalyst and/or sorbent particles. The reactor has three thermocouple ports to monitor the bed temperature and is located inside a tube furnace. A back pressure regulator is used to control the adsorption pressure (as needed). After exiting the reactor, the major synthesis components CO, H₂, CH₄ and CO₂ content of the stream are monitored by an on-line NOVA Multi-gas Analyzer and humidity probes are used to measure the inlet and exit humidity levels. Continuous analysis of CO and CO₂ in the exit gas allows us to monitor breakthrough gas concentrations and to measure a total CO conversion and CO₂ adsorption capacity. The apparatus is fully automated and can run without an operator for long periods of time, including overnight. The control system controls the test conditions, logs the analytical data, and also safely shut down the apparatus in case of a malfunction.

3.2.2 WGS Catalyst Evaluation

Initially, we carried out cycling tests with WGS catalyst alone to establish a baseline CO conversion at lower Steam: CO ratios of 1.5 and 1.2. In these experiments we tested both commercial WGS catalyst and TDA's contaminant tolerant WGS catalyst. The Sud-Chemie's ShiftMax®-230 catalyst showed almost similar conversions (less than the equilibrium) for steam: CO ratios of 1.2 and 1.5 (Figure 8). Higher temperatures provided higher conversions and the conversions approached closer to equilibrium.

Figure 8. CO conversion under different steam: CO ratios and temperatures for commercial WGS catalyst (Shiftmax-230) at 500 psig.

We then carried out cycling tests with TDA's WGS catalyst (based on Pt/CeO₂) that is contaminant tolerant. The catalyst achieved lower CO conversions than the commercial catalyst and the conversions increased at higher temperatures (Figure 9). However, higher temperature operation results in lower equilibrium CO conversion and CO₂ capacity. Hence, we selected Shiftmax®-230 for our combined WGS catalyst and CO₂ sorbent tests.

Figure 9. CO conversion at different temperatures, 500 psig and steam: CO ratio of 1.5 for TDA's contaminant tolerant WGS catalyst (Pt/CeO₂).

The platinum-ceria catalyst was developed by TDA under a DOE SBIR Phase I project (DE-SC0004379) as a contaminant tolerant water gas shift catalyst and under that DOE project it was extensively evaluated under the presence of different contaminants that could be present in the synthesis gas. However, in this project the platinum-ceria catalyst is found to be more active only at temperatures in excess of 300°C while the CO₂ sorbent is effective at temperatures below 300°C. Hence, in this project, we have decided to use the commercial water gas shift catalyst such as the low temperature shift catalyst (Shiftmax-230 from Sud-Chemie). This catalyst is similar to that used in the DOE modeling study (DOE/NETL – 2007/1281) for IGCC systems with CO₂ capture. The Water gas shift system is located downstream of the gas cleanup that removes H₂S and COS. Hence, the only contaminants that may come into contact with our system are the heavy metals such as arsenic and mercury. In a DOE SBIR Phase II project (Contract # DE-FG02-08ER-85211) we are developing a multi-contaminant control system that uses similar mesoporous carbons as supports where the mesoporous carbons are incorporated with surface functional groups for removing the heavy metals (arsenic, mercury and selenium). These metals are retained by the sorbent at temperatures up to 300°C. Arsenic is present as arsine in the synthesis gas and remains in the gas phase during warm gas capture of CO₂ without condensation on CO₂ capture equipment and sorbent. The CO₂ sorbent has some capacity for Hg and will remove Hg during CO₂ capture, however the Hg is not released under pressure swing from our sorbent surface.

Table 3. Simulated un-shifted synthesis gas with H₂O: CO = 1.5:1

gas	vol. %
CO ₂	14
CO	37
H ₂	26
N ₂	8
H ₂ O	53

T = 240°C; P = 500 psig

3.2.3 Combined WGS Catalyst and CO₂ Sorbent Evaluation

We initially mixed the catalyst (ShiftMax®-230) into the TDA's CO₂ sorbent (AMS-19) at 10% by vol. and carried out multiple pressure swing adsorption cycles using simulated un-shifted synthesis gas at bench-scale. The composition of the synthesis gas used is provided in Table 3. Figure 11 and Figure 10 shows the CO and CO₂ breakthrough under cycling. We did not observe any CO breakthrough during either the adsorption or desorption steps, indicating that there

Figure 10. Combined WGS and CO₂ capture with 10% (vol.) Shiftmax 230 in TDA's CO₂ sorbent – AMS-19. CO₂ in the feed and product. is complete conversion of CO present in the feed to CO₂. The sorbent achieved a total CO₂ loading of 7.82% wt. of which 5.68% is from conversion of CO into CO₂, with the remainder of the adsorbed CO₂ coming from the CO₂ in the feed stream.

Figure 11. Combined WGS and CO₂ capture with 10% (vol.) Shiftmax 230 in TDA's CO₂ sorbent – AMS-19. CO in the feed and product.

We then carried out cycling tests with different catalyst/sorbent ratios (for e.g., 1%, 4%, 6%, 7%, 10% by vol.) and at different steam: CO ratio 1.2 to 1.5 using both un-shifted and pre-shifted synthesis gas. When we carried out tests with a lower catalyst to sorbent ratio of 1% by vol. using un-shifted synthesis gas, it resulted in CO leakage. So we carried out tests with lower catalyst to sorbent ratios using partially shifted synthesis gas. Table 4 shows the composition of the partially shifted synthesis gas mixture used in the bench-scale tests. We mixed 6% by vol. WGS Catalyst (ShiftMax®-230) with our CO₂ removal sorbent in a 100 mL reactor and carried out tests at 240°C and 500 psig pressure using pre-shifted synthesis gas at different steam: CO ratio. The CO conversion was 90+% for Steam: CO ratios 1.28 and above as shown in Table 5. These tests were carried out with the sorbent being saturated with CO₂.

Table 4. Simulated partially shifted synthesis gas with H₂O: CO = 1.5:1 inlet to 1st stage WGS.

Gas	Vol. %
CO ₂	29.5
CO	3.6
H ₂	37.1
N ₂	3.1
H ₂ O	26.2

Table 5. CO conversion as a function of Steam: CO ratio for a 6% vol. catalyst mixed with CO₂ sorbent bed at T = 240°C and P = 500 psig.

Steam:CO Ratio	CO Conversion (%)
0.77	1%
1.02	79%
1.28	91%
1.54	92%

Figure 12. Combined WGS and CO₂ capture with 6% (vol.) Shiftmax 230 in TDA's CO₂ sorbent – AMS-19. CO in the feed (partially shifted synthesis gas) and product at different H₂O flow rates (i.e., steam: CO ratio).

3.2.4 Characterization of Tested Samples

We carried out characterization of the tested samples, i.e., the ShiftMax®-230 catalyst and the TDA's CO₂ sorbent (AMS-19) that has been cycled for over 100 cycles at temperature and pressure in the presence of simulated synthesis gas. We compared the characterization results against the fresh samples to understand any chemical changes that may have occurred due to cycling them under the combined WGS and CO₂ capture conditions. The tested samples of the sorbent and catalyst maintained their surface area and we also measured the X-ray diffraction pattern for the WGS catalyst. The catalyst maintained its crystallinity and there no extra peaks in the XRD indicating that there were no chemical changes to the catalyst surface due to cycling under combined WGS and CO₂ capture conditions. The CO₂ sorbent is amorphous and the XRD confirmed the same after testing. Table 6 shows the summary of the surface area of the fresh and tested samples of catalyst and sorbent. Figure 13 shows the XRD patterns for the fresh and tested catalyst sample (taken after regeneration step) and CO₂ sorbent.

Table 6. BET Surface area of the fresh vs tested samples.

Sample	BET Surface Area (m ² /g)	
	fresh	tested
CO ₂ Sorbent (AMS-19)	453	448
WGS Catalyst (ShiftMax®-230)	93	77

We also carried out characterization of the tested sample after the adsorption step. Figure 14 shows the XRD of the tested catalyst after adsorption step, which retained its Cu and Zn peaks and the peaks were much sharper and more prominent.

Figure 13. XRD patterns of fresh and tested WGS catalyst (ShiftMax®-230) and CO₂ sorbent (AMS-19).

Figure 14. XRD of the tested low temperature shift catalyst (ShiftMax®-230).

3.3 Task 3. Multiple Cycle Tests

In this task, we carried out multiple cycling experiments under pre-shifted simulated synthesis gas to assess the impact on sorbent's CO₂ capacity and effectiveness of WGS catalysts for CO conversion. The sorbent and catalyst maintained their CO₂ capacity and CO conversion over 1,140 cycles.

We carried out multiple cycle tests using a catalyst/sorbent ratio of 10% by vol. in a split bed configuration (Figure 15). The tests were carried out in a 100 mL bed with partially shifted synthesis gas (47.2% H₂, 4.6% CO, 37.6% CO₂, 10.6% N₂ on dry basis). We completed over 1,140 cycles and the CO₂ capacity of the sorbent/catalyst combination over 1,140 cycles is reported in Figure 16 for the pre-shifted synthesis gas when a Steam: CO ratio of 1.5 is used in the first WGS stage. The sorbent maintained a capacity of 6.5% wt. CO₂. Figure 17 shows the CO₂ and CO breakthrough during these cycle tests. We removed all of the CO₂ and the CO during the adsorption step and most of the CO removed is converted to CO₂ which is shown in Figure 18. The CO conversion was stable,

Figure 15. We carried out multiple cycle tests in a split bed configuration as illustrated above.

Figure 16. CO₂ capacity of the sorbent in multiple pressure swing cycles tests in a split bed configuration.

Figure 17. CO₂ and CO breakthrough in the multiple cycle tests in a split bed configuration. staying above 73%.

Figure 18. CO conversion of the catalyst in multiple pressure swing cycles tests in a split bed configuration with partially shifted synthesis gas.

3.4 Task 6: Modification of the Prototype Test Unit

In this task we carried out modifications to a 4-bed high temperature pressure swing adsorption (PSA) prototype test system and the integrated gas conditioning skid, the unit was fabricated earlier under a previous DOE NETL funded project (DE-FE-0000469). In the previous project, we had successfully demonstrated the CO₂ capture performance of the 4-bed high temperature PSA prototype test unit at National Carbon Capture Center (NCCC – Wilsonville, AL) and the Wabash River IGCC plant (Terra Haute, IN) using TDA's CO₂ sorbent under actual coal derived syngas synthesis gas. T

The test unit consists of two parts, the Gas Conditioning Unit and the PSA CO₂ Adsorption Unit. As shown in Figure 19, synthesis gas (Stream 1.0) enters the Gas Conditioning Unit (GCU) where it flows through a sulfur removal bed to eliminate sulfur bearing contaminants. Next, the gas is mixed with steam produced by the GCU and enters a reactor containing water gas shift catalyst. Water gas shift takes place in order to either fully or partially shift the CO rich synthesis gas (less than 90% CO conversion) to CO₂ and H₂ before entering the PSA Unit. Once in the PSA Unit, the gas flows through one of the four sorbent containing packed beds while the other three beds are either depressurizing or being regenerated using a nitrogen stream. Two NOVA flue gas analyzers measure the concentrations of CO₂, CO and H₂ in both the syngas exit stream as well as the regeneration stream.

Average Flows		CO Conversion		88.8%	96.7%	S/CO ratio		1.15			
Stream	1.0	1.1	1.2	1.3	1.4	1.5	2.0	3.0	3.1	3.2	4.0
gmol/hr											
H ₂ O	15.1	15.1	31.4	7.2	7.2	37.9	0.0	16.3	16.3	16.3	37.9
H ₂	18.1	18.1	18.1	42.4	41.1	1.3	0.0	0.0	0.0	0.0	0.0
H ₂ S	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
CO	27.3	27.3	27.3	3.1	0.9	2.2	0.0	0.0	0.0	0.0	0.0
CO ₂	10.5	10.5	10.5	34.8	0.3	34.4	0.0	0.0	0.0	0.0	0.0
N ₂	1.8	1.8	1.8	1.8	0.0	1.8	0.0	0.0	0.0	0.0	0.0
Other	2.0	2.0	2.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
Total	75.8	74.8	91.2	91.2	51.5	77.6	1.0	16.3	16.3	16.3	37.9
Temp	C	193.8	250.0	293.8	350.0	110.0	85.0	20.0	20.0	350.0	25.0
Press	PSIG	357.0	356.0	356.0	356.0	1.5	2.0	50.0	450.0	450.0	100.0

Figure 19. Prototype Test Unit PFD and stream data.

The high temperature PSA CO₂ removal system consists of four packed beds filled with TDA's CO₂ sorbent. This allows for continuous product flow through the system. The bed and valve layout was designed around the cycle sequence shown in Figure 20. Each bed has three valves on the inlet and two valves on the outlet to allow for continuous product flow during bed regeneration and depressurization. A four bed system increases the hydrogen

	Stage 1			Stage 2			Stage 3			Stage 4		
Time (min)	11			2	7	2	2	7	2	2	7	2
Bed 1	ADS			EQ1	HOLD	EQ2	BD	PURGE	EQ3	EQ4	HOLD	PRESS
Bed 2	EQ4	HOLD	PRESS	ADS			EQ1	HOLD	EQ2	BD	PURGE	EQ3
Bed 3	BD	PURGE	EQ3	EQ4	HOLD	PRESS	ADS			EQ1	HOLD	EQ2
Bed 4	EQ1	HOLD	EQ2	BD	PURGE	EQ3	EQ4	HOLD	PRESS	ADS		

4- bed PSA Cycle Steps	
Step 1	Adsorption at 500 psig (ADS)
Step 2	Pressure Equalization to 383 psig (EQ1)
Step 3	Hold at 383 psig (HOLD)
Step 4	Pressure Equalization to 267 psig (EQ2)
Step 5	Blowdown to 150 psig (BD)
Step 6	Steam Purge at 150 psig (DES)
Step 7	Pressure Equalization to 267 psig (EQ3)
Step 8	Pressure Equalization to 383 psig (EQ4)
Step 9	Hold at 383 psig (HOLD)
Step 10	Pressurization with feed to 500 psig (PRESS)

Figure 20 PSA 4 Bed Cycling Sequence for 500 psig operation.

recovery of the system by allowing the low pressure regenerated bed to partially pressurize with the high pressure bed that has just finished with adsorption step. This occurs during the equalization step of the sequence. In the combined WGS and CO₂ removal tests three out of the four beds were filled with a mixture of WGS catalyst and sorbent.

The P&ID of the PSA CO₂ Removal Unit is shown in Figure 21. The partially shifted and sulfur

Figure 21 CO₂ Adsorption Unit P&ID

free syngas enters the system and is diverted to any of the four beds depending on the orientation of the valves located at the bottom of each reactor vessel. All the gas lines in the system are heat traced and all the valves are located in metal boxes that are heated beyond the dew point of the gas in order to prevent water and hydrocarbons from condensing in the piping and on the sorbent. To keep the beds hot, each reactor is wrapped in a heated and insulated jacket and the vessel surface temperature is precisely controlled. After adsorption, the CO_2 the WGS equilibrium shifts and allows for more conversion of CO resulting in an (almost) carbon free syngas flow into the accumulator vessel (R-100). The volume of the accumulator is approximately four times that of the reactors. Its purpose is to pressurize the reactors with CO_2 free syngas once regeneration and equalization has taken place. Flow out of the system is controlled by a Badger Research Control Valve and flow rate is measured by a turbine flow meter.

Figure 22 Valve Box Layout

Once a bed is close to its breakthrough for CO_2 , the next step is to “blow down” or depressurize the bed rapidly to help drive off the CO_2 that is adsorbed on the surface of the sorbent. Once the bed reaches approximately 75 psig, heated nitrogen is sent through the bed from the top down to continue to drive off the remaining CO_2 adsorbed on the surface of the sorbent. A Badger Research Control Valve controls the flow of nitrogen along with the rate in which the bed depressurizes. A mass flow meter measures the amount of nitrogen that is sent through the bed. A turbine flow meter measures the combined outlet flow to help determine the amount of the CO_2 and H_2 that is in the regeneration stream.

Gas sampling is taken at multiple points in the system. A sample stream is taken from the syngas outlet and sent to a gas analyzer which is capable of determining the concentrations of CO_2 , CO and H_2 . Samples can be taken before or after the accumulator in order to analyze the performance of each individual bed or the entire system. A sample stream is also taken from the regeneration side and sent to a NOVA analyzer to determine its CO_2 , CO and H_2 content.

Before entering the CO_2 adsorption unit, the syngas is first processed by the gas conditioning unit. As shown in the P&ID (Figure 23), the syngas first passes through either R-203 or R-204. Both reactors contain Actisorb®, a sulfur removing sorbent. Two identical reactors are used so that once one bed is spent, flow is diverted to the other bed with minimal interruption of operation. Both vessels are internally heated using cartridge heaters. After desulfurization, steam is added to the syngas to raise the steam:carbon ratio in order to perform water gas shift. Water is pumped into a heated $\frac{1}{4}$ ” line and is vaporized. A Badger Research Control Valve maintains slightly higher pressure in the steam generation line to ensure that the steam entering the syngas is completely vaporized. The syngas and steam mixture travels to R-220 which contains the water gas shift catalyst Shiftmax® 240. This copper based catalyst performs the water gas shift reaction, $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$. The remaining CO content in the outlet stream is monitored to ensure that there is enough steam to not only shift the CO but to prevent coking of the catalyst. The shifted syngas then exits the gas condition unit via a heated gas line to the CO_2 adsorption unit. In the case of combined WGS and CO_2 removal tests the shift reactor was

Figure 23 Gas Conditioning Unit P&ID

operated with minimum Steam:CO ratio such that CO is only partially shifted in this step and the rest is shifted in the CO₂ removal step.

Safety: Test Unit had previously passed a thorough Process Hazard Analysis (PHA) at the Wabash River IGCC plant and the NCCC to ensure the all aspects of the Test Unit are safe for operation and complies with onsite rules and regulations. A safe operating procedure was also developed to ensure that safe operation of the test unit is always followed. Both units are housed in NEMA enclosures (Figure 24), which will be purged with nitrogen in accordance with standard Class I Division II practices. Purge monitors will measure the pressure created by the purge and will shut the system down if there is insufficient flow to the enclosures. Steam rated pressure relief valves are located throughout the entire test unit in order to prevent over-pressurization of the vessels and tubing. Pressure throughout the entire unit is monitored using a series of pressure transducers. Each pressure measurement is associated with a software interlock which will shut the system down if the measured pressure exceeds a predetermined set point. Every heater in the system is monitored by two thermocouples. One is wired directly to an over-temperature module which will terminate power to all heaters if the measured temperature exceeds the set point on the module. The other thermocouple is wired to the Labview control software which is used for control. The software will shut the system down if the monitored temperature exceeds the predetermined set point. Combustible gas monitors are located in both cabinets to monitor possible leakage inside the enclosures. A shutdown will be initiated if the amount of combustible gases exceeds a safe level within the enclosure. All the fittings and tubing are rated well above the maximum limit of the apparatus for pressure and

temperature ratings. All fittings used in high pressure and temperature regions are Swagelok® compression fittings. Each vessel is ASME rated for well above the temperatures and pressures of the system.

Figure 24. CO₂ Adsorption Unit (Left) Gas Conditioning Unit (Right)

Modifications to the Prototype Unit: The CO₂ sorbent from Beds 1-3 was removed and mixed with Süd-Chemie Shiftmax® 120, a low temperature copper-zinc based WGS catalyst. The beds were filled in 3 sections as shown in Figure 25. The syngas enters the bed where CO₂ is initially removed in the sorbent only section. This will help drive the water gas shift reaction further to completion once the syngas reaches the mixed catalyst and sorbent section of the bed. To help prevent CO₂ leakage, the syngas will flow through another sorbent only section to adsorb any remaining CO₂ generated from the water gas shift section. The reactor end caps on either end are filled with inert 1/8" Denstone® pellets. Bed 4 was filled with the same amount of the sorbent as Beds 1-3 with rest inert Denstone® and will be used as a control in the demonstration testing. The sorbent used in all the beds is the same sorbent as used in the previous two testing campaigns.

Figure 25. We filled the sorbent beds in the configuration shown above.

Modifications were done to the gas sampling system as well: rotameters and gas desiccant beds were moved to the outside of the enclosure in order to closely monitor flow and allow for easier desiccant changes. Three of the high temperature valves were also rebuilt due to leakage.

3.5 Task 7: Field Demonstration

The modified prototype unit was shipped from Wabash River IGCC to the Wilsonville NCCC during the week of March 11, 2013. It was installed during the week of March 18 (Figure 16). From March 25-27, 2013, the unit underwent shakedown tests and programming changes. The field tests started on March 27, 2013 with the unit receiving syngas at about 3 lbs/hr (~ 1 scfm) at 250°C and 200 psig.

Figure 26. Field demonstration unit installed at the NCCC in Wilsonville, AL

One of the first objectives in this field test was to determine the gas composition that is entering the sorbent beds post WGS that is located in the gas conditioning unit. Syngas was flowed through the system at steam:CO ratios from 1.1 to 3. Flow was sent through bed 4 until the sorbent was saturated and the outlet compositions were measured. Using NCCC's inlet gas composition it was determined that the WGS reactor was only converting between 15-17% of the CO. This could be due to deactivation of the catalyst during the previous testing campaign due to coking and sulfur poisoning. Regardless, this was ideal in order to determine the performance of the catalyst residing in the beds. Table 7 shows the gas compositions entering the unit from NCCC and the gas compositions entering the sorbent beds.

Table 7. Gas Compositions.

	From NCCC	Inlet To Sorbent Beds
H ₂ O	7.9%	7.5-8.6%
H ₂	6.1%	7.3%
CO	9.0%	7.0%
CH ₄	0.9%	0.9%
CO ₂	8.0%	9.7%
N ₂	68.0%	68.0%

The next series of tests involved running single bed saturation cycles to determine the sorbent's CO₂ capacity and the catalysts CO conversion percentage. Figure 27 shows the outlet CO₂ and CO compositions for each bed cycle. The green line represents the amount of CO that is in the regeneration stream which is the amount of CO that is picked up by the sorbent and is not

Figure 27. Single Bed Cycle outlet gas composition

converted. To determine the CO conversion for beds 1-3, the CO coming out in the regeneration and clean-CO₂ free syngas streams were integrated and subtracted from the inlet CO flow rate. The CO₂ sorbent capacity was calculated similarly with the CO₂ in the outlet integrated and subtracted from the inlet CO₂ and then normalized by the mass of CO₂ adsorbed by the weight of the sorbent. As shown by graph, the CO in the outlet of beds 1-3 is near nonexistent while the CO in the outlet of bed 4 which contains no catalyst reaches the inlet CO concentration.

Figure 28. Sorbent Bed CO conversion in comparison to equilibrium CO conversion at 230°C at different S/CO ratios

The CO conversion and weight capacity were averaged for each bed. As shown in Figure 28, the CO conversion at a steam:CO ratio of 1.1 is over 5% more than that what is predicted by the WGS reaction equilibrium at a temperature of 230°C and 200 psig. This shift in equilibrium is most likely due to the closely coupled removal of the product gas, CO₂ which enables the reaction to reach closer to completion. The CO conversion at a steam:CO ratio of 1.0 is lower than equilibrium; this is most likely due to the sorbent section, which occupies the initial 20% of the bed at the syngas inlet, some of the water is picked up at the inlet section (this water pick up is due to the use of nitrogen instead of steam during regeneration, else the bed during a typical cycle will neither pick up nor release water during both adsorption and desorption) and prevents the catalyst section from fully seeing the stoichiometric amount of steam, resulting in lower than equilibrium conversion. There is unreacted CO that is trapped in the voids in this initial sorbent section that can be seen immediately on the regeneration cycle (Figure 27). Adding a small portion of catalyst in this section of the bed may reduce this and will also drive the conversion higher at the lower steam:CO ratios.

Figure 29. Sorbent CO₂ capacity at varying steam:CO ratios.

The CO₂ capacity was calculated at varying steam:CO ratios and the averages shown in Figure 29. The capacity of the sorbent is slightly higher than the last campaign at steam:CO ratios between 1 and 1.5. The increase in CO₂ capacity is most likely due to the decrease in H₂O in

the feed stream which raises the CO_2 partial pressure. At steam:CO ratio of 2.0, which is same as previous test campaign the sorbent capacity was lower.

Figure 30. Carbon capture rates during a portion of testing.

In this test campaign the system was online for over 600 hours during which approximately 32,000 SCF of syngas was processed. Figure 30 shows the amount of total carbon entering the prototype unit as CO and CO_2 and the amount of carbon exiting the apparatus along with the high pressure syngas.

The average overall carbon capture rate for this demonstration test campaign was over 96% with an average overall CO conversion of 96.4% at an average steam:CO ratio of 1.1.

An important observation during these tests was that the bed temperature was higher when the catalyst and sorbent operated together compared to previous test campaigns with only the CO_2 sorbent.

Figure 31 shows the temperature rise for the sorbent only case and the combined catalyst and sorbent case. As expected, temperature increase was much higher when the WGS reaction was combined with the CO_2 removal. The heat effects will be more pronounced with higher CO/ CO_2 content synthesis gas (as mentioned the NCCC gas was diluted with nitrogen due to the air blown transport gasifier used for gasification of the coal).

Figure 31. Temperature difference during adsorption for sorbent only and mixed sorbent/catalyst bed.

3.6 Task 4. Process Design and Modeling

In this task, TDA, in collaboration with Phillips 66 and UCI performed a detailed process design and modeling using Aspen-PlusTM simulation software to calculate material and energy balances of an advanced pre-combustion carbon system that combines simultaneous shifting of the syngas and CO₂ capture using a combination of WGS catalyst and TDA's CO₂ sorbent that selectively removes CO₂ above the dew point of the synthesis gas with an E-GasTM gasifier based IGCC power plant operating on low rank coals. The sorbent regeneration is carried out using a combination of pressure swing (i.e., reducing the pressure to 10 barA) and concentration swing by using steam purge per regeneration while maintaining near isothermal operation. The near isothermal conditions are maintained by equipping the vessels with internal heat transfer tubes that generate steam. The high temperature pressure swing adsorption (PSA) unit also removes trace metal contaminants (such as Hg and As) and when combined with warm gas desulfurization cleanup provides a complete warm gas clean-up platform for IGCC plants. For a nominal 600 MW IGCC plant, the CO₂ removal system consists of three trains of 8-bed shift/PSA units (total of 24 beds housing the shift catalyst and the CO₂ sorbent) that undergo a PSA sequence, including adsorption, depressurization, pressure equalization, desorption and steam purge; all of which ensure continuous removal of CO₂ from the synthesis gas, generating a concentrated CO₂ stream ready for further purification and compression and also a very low CO₂ containing synthesis gas fuel to be combusted in the gas turbine. Consistency has been maintained between the IGCC case developed under this study utilizing the TDA's regenerable sorbent CO₂ capture process (Warm Gas Cleanup Case) with the Phillips 66 (E-GasTM) gasifier based IGCC with CO₂ capture utilizing current state-of-the-art SelexolTM based syngas cleanup and CO₂ capture technology (Cold Gas Cleanup Case) that makes up Case S4B in the DOE NETL study report DOE/NETL-2010/1399 titled, "Cost and Performance Baseline for Fossil Energy Plants Volume 3a: Low Rank Coal to electricity: IGCC Cases," dated May 2011.

3.6.1 Task 4.1 Design of Combined WGS and PSA System

Figure 32. Typical cycle scheme for pre-combustion CO₂ capture that includes four pressure equalization steps with a co-current blowdown step to improve the H₂ and CO₂ recoveries.

We used computer simulation program that uses mathematical models to represent each of the pressure swing adsorption (PSA) cycle steps. This model assumes axial dispersed plug flow of a binary gas mixture through a packed adsorbent bed with spherical adsorbent particles (H₂, CO₂). We have used the parameters obtained from the Field tests for CO conversion obtained in the combined WGS and CO₂ capture beds to carry out the binary simulations. Figure 32 shows a typical PSA cycle scheme with three pressure equalizations for pre-combustion CO₂ capture system using TDA's sorbent. An important observation during the field test campaign

was that the bed temperature was higher when the catalyst and sorbent operated together. Figure 31 shows the temperature rise with the sorbent only case and when the bed has both the sorbent and the catalyst. As expected, temperature increase was much higher when the WGS reaction combined with the CO₂ removal. The heat effects will be more pronounced with higher CO/CO₂ content synthesis gas (the synthesis gas in the NCCC demonstration was diluted with nitrogen from the air blown gasifier).

Figure 33. Temperature difference during adsorption for sorbent only and mixed sorbent/catalyst bed.

Hence, we decided to combine just the last stage of WGS to minimize the heat release from the beds. This could also be used to minimize or eliminate the steam addition, depending on the coal type. In the case of low rank coals such as lignite there is excess water in the synthesis gas (3.12 steam to CO ratio). Hence the benefit of reduced steam consumption would not be realized in the case of low rank coals. When combining just the last stage of WGS the heat release from the shift reaction is used to raise steam while the heat release from the CO₂ adsorption is just stored in the sorbent bed and is used for desorption.

In our design, we looked at various options for heat transfer such as removing the heat by adding steam directly into the CO₂ scrubber/WGS reactor. The direct evaporation of water in the reactor represents the most efficient method of heat extraction (e.g., in comparison to indirect heat exchangers that boil water inside the tubes embedded into the sorbent/catalyst bed). The synthesis gas temperature will be immediately reduced when it is in contact with the evaporator. Our calculations suggest a good match for the amount of heat extracted from the unit and the amount of heat released by the WGS processes.

Figure 34. Schematic of potential design of the combined WGS/CO₂ capture PSA bed (reactor).

We envision a simple design for the CO₂ scrubber/WGS reactor that resembles a shell and tube heat exchanger. The sorbent and catalyst pellets will be packed into the shell-side, while high pressure water will continuously feed into the tube side (various designs will be considered with a dead-ended tube or a flow through system). The filter tubes of 0.5" OD and 2.4 m (8.0 ft) length are welded to a tube sheet with proper manifolding (longer dimensions by combining the tubes with unions is possible). The proposed design to control temperature rise in the fixed beds is very straight forward.

Figure 34 shows a schematic of a potential design of the CO₂ scrubber/WGS reactor with cooling tubes for heat exchange. The synthesis gas flows from top down, first across a sorbent top layer to remove CO₂ (to shift the equilibrium of the gases), which will allow the catalyst to shift CO as soon as the gas enters into the subsequent mixed sorbent/catalyst layer. In this mixed bed, cooling tubes are placed to provide cooling. Alternatively we also looked at steam injection with direct evaporative cooling where the injection rate of the steam matches the rate of disappearance of steam via the WGS reaction. The heat balance works well; for every mole of steam introduced into the system, 11 kcal/mole will be extracted (to generate steam from 50°C water), while each mole of steam consumed by the WGS reaction will release 9.8 kcal/mole. This good match in heat of reaction and evaporation will provide good control of temperature in the reactor. A layer of sorbent bed follows the mixed catalyst/sorbent to scrub out any remaining CO₂. In our approach we will restrict the amount of heat removal to match the heat released by the WGS process and not the heat of CO₂ removal (every mole of CO₂ adsorbed by the sorbent will also generate 4.9 kcal/mole) as this heat will be removed during the regeneration process, when CO₂ is released (in the overall process with the proposed cooling approach, the bed temperature will increase from 220 to 230°C during adsorption, and the bed will cool down back to 220°C at the completion of the sorbent regeneration).

We also explored advanced design concepts for steam introduction that could potentially provide better heat management and allow more of the WGS reaction to take place in the sorbent bed. However, a more thorough evaluation of various heat transfer design options and the optimization of CO conversion that is allowed to happen in the combined WGS and CO₂ capture beds are needed, but are beyond the scope of this project. We have subsequently been awarded a new DOE contract (DE-FE-0012048) where we will carry out detailed CFD modeling of the shell and tube heat exchange porous stainless membrane reactors for the combined WGS and CO₂ capture above the dew point of the syngas using TDA's CO₂ sorbent.

Hence in this project, we decided to combine just the last stage of WGS to minimize the heat release from the beds while heat transfer is still accomplished by shell and tube heat exchange stainless tubes (This type of internally cooled fixed bed reactors are common in industry). The amount of heat that will be released in the combined WGS and CO₂ capture beds, if we conduct the entire WGS in the PSA beds is approximately three times the heat release for a simple PSA bed removing just the CO₂ after carrying out two or three-stage WGS reaction upstream. When combining just the last stage of WGS the heat release from the shift reaction is used to raise steam while the heat release from the CO₂ adsorption is just stored in the sorbent bed and is used for desorption.

In order to incorporate the last stage of the water gas shift reaction in the PSA model, we assumed that WGS reaction proceeds to 96.4% overall completion when exiting the PSA beds and additional heat generated from the exothermic WGS reaction has been assumed to be removed by using internal cooling tubes where we generate steam i.e., the sorbent bed will retain the heat of CO₂ adsorption, which will be consumed during desorption, while the heat generation from WGS is constantly removed using internal heat exchanger tubes incorporated into the fixed bed reactors. The sorbent bed is assumed to be non-isothermal and the external film diffusional resistance is assumed to be negligible compared to the resistance in the pores of the sorbent. The axial pressure drop is neglected and gases are assumed to be ideal. The equilibrium relations for both the components are represented by extended binary Langmuir-Freundlich isotherms. The average diffusional time constants are estimated from the bench-scale kinetic data from the isotherm unit. The exponential pressure profile (history) is assumed for the variable pressure steps with the time constant chosen according to the thumb rule

described by Farooq et al. (1993). The model equations for isothermal conditions are shown below and more details about the model and computer simulations can be found in the Ph.D. dissertation by Jayaraman (2004).

The fluid phase mass balance for component k is given below:

$$\varepsilon_t \frac{\partial y_k}{\partial t} - \varepsilon D_{ax} \frac{\partial^2 y_k}{\partial z^2} + \varepsilon \frac{\partial (u y_k)}{\partial z} + \frac{\rho_b RT}{P} \frac{\partial \bar{q}_k}{\partial t} + \frac{\varepsilon_t y_k}{P} \frac{dP}{dt} = 0 \quad (1)$$

The overall material balance is given by:

$$\varepsilon \frac{\partial u}{\partial z} = - \frac{\rho_b RT}{P} \sum_{k=1}^2 \frac{\partial \bar{q}_k}{\partial t} - \frac{\varepsilon_t}{P} \frac{dP}{dt} \quad (2)$$

The particle phase mass balance for component k as given by the intraparticle diffusion equation for a sphere:

$$\frac{\partial q_k}{\partial t} = \frac{D_{e,k}}{r^2} \frac{\partial}{\partial r} \left(\frac{1}{r^2} \frac{\partial q_k}{\partial r} \right) \quad (3)$$

with boundary conditions:

$$\frac{\partial q_k}{\partial r} = 0 \quad \text{at } r = 0 \quad (4)$$

$$-D_{e,k} \frac{\partial q_k}{\partial r} \bigg|_{r=R} = a_k (q_k|_{r=R} - q_k^*) \quad \text{at } r = R \quad (5)$$

where q_k^* is the equilibrium amount adsorbed at the surface of the crystal and can be calculated using the extended binary Langmuir-Freundlich isotherm:

$$q_k^* = \frac{q_{mk} B_k P_k^{n_k}}{1 + \sum_{j=1}^2 B_j P_j^{n_j}} \quad (6)$$

The volume averaged adsorbed phase concentration $\bar{q}_k$ is given by

$$\bar{q}_k = \frac{3}{R^3} \int_0^R q_k r^2 dr \quad (7)$$

The boundary conditions for the fluid phase mass balance are given below for Cycle (I):

(1) Pressurization Step:

$$\text{at } z = 0, \quad y_k = y_{f,k}$$

$$\text{at } z = L, \quad u = 0$$

$$P = P(t) = P_{DES} + (P_H - P_{DES}) (t/\square_p)$$

$$D_{ax} \frac{\partial y_k}{\partial z} \bigg|_{z=0} = u_H (y_k|_{z=0} - y_{H,k}) \quad (8a)$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=L} = 0 \quad (8b)$$

(2) High Pressure Feed Step:

$$\text{at } z = 0, \quad y_k = y_{f,k} \quad u = u_f$$

$$P = P_H$$

$$D_{ax} \left. \frac{\partial y_k}{\partial z} \right|_{z=0} = u_H (y_k|_{z=0} - y_{H,k}) \quad (9a)$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=L} = 0 \quad (9b)$$

(3) Cocurrent depressurization Step:

$$\text{at } z = 0, \quad u = 0$$

$$P = P(t) = P_{COBD} + (P_H - P_{COBD}) (t/\tau_{codb})$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=0} = 0 \quad (10a)$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=L} = 0 \quad (10b))$$

(4) Countercurrent Blowdown Step:

$$\text{at } z = L, \quad u = 0$$

$$P = P(t) = P_{CBD} + (P_H - P_{CBD}) (t/\tau_{bd})$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=0} = 0 \quad (11a)$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=L} = 0 \quad (11b)$$

(5) Countercurrent Desorption / Purge Step:

$$\text{at } z = L, \quad y_k = y_{p,k}$$

$$\text{at } z = L, \quad u = u_L$$

$$P = P(t) = P_{DES} + (P_{CBD} - P_{DES}) (t/\tau_{des})$$

$$-D_{ax} \left. \frac{\partial y_k}{\partial z} \right|_{z=L} = u_L (y_{L,k} - y_L|_{z=L}); (u_L < 0) \quad (12a)$$

$$\left. \frac{\partial y_k}{\partial z} \right|_{z=0} = 0 \quad (12b)$$

The above partial differential equations were solved by an implicit finite difference method using a Crank-Nicolson scheme. In the simulation 100 grid points are used in the bed with the convergence criterion set at 1×10^{-3} . The FORTRAN PSA simulation code developed by Sun et al. (1996) is used. In most simulations the steady state was reached within 50 cycles, so carried out simulations up to 100 cycles (Figure 35).

Table 8 shows the list of the parameters used in the binary simulations, which were later extended to full-scale system. Figure 36 shows the gas phase H_2 wave fronts as it travels (from left to right) through the sorbent bed during the course of the Feed (adsorption) step. Similar wave fronts are calculated for each of the steps for both H_2 and CO_2 . The computer simulations provides the bed profiles at various steps in the PSA cycle and can be used to optimize the step times, step pressures and purge volumes etc. We initially verified the model results against the CO_2 working capacity from our bench-scale tests, which were carried out with a simple 4-step PSA cycle consisting of pressurization, high pressure feed/adsorption step, blowdown and purge and the results are reported in Table 9. The CO_2 working capacity calculated by the mathematical model based computer simulations for a simple 4 step cycle is 7.3% wt. CO_2 , which is similar to the results obtained in the long-term cycling results.

Table 8. Summary of simulation parameters used.

Sorbent Bed Parameters

Bed Length	0.51 meters
External Porosity	0.4
Radius of the Adsorber	0.0635 meters
Bed (L/D)	4.0
Bed Density	354 kg/m ³
Shape of Pellets	spherical
Pellet Porosity	0.57
Radius of Pellets	3.0E-04 meters
Number of Grids in the Bed	100
Axial Dispersion Coefficient	5.38E-06 m ² /sec
Heat Capacity of the Bed	930 J/kg/K
Effective Heat Conductivity	0.11 W/m/K
Heat Transfer Coefficient	5 W/m ² /K
Wall Temperature	240 °C

CO_2 Adsorption Parameters

Langmuir Coefficient (q_s)	386.4 mmol/g
Langmuir Coefficient (B)	4.15E-04 1/atm
Langmuir Coefficient (n)	0.869
Diffusion Coefficient (D/R^2)	1.32E-03 1/s
Reference Temperature for B	240 °C
Heat of Adsorption (ΔH)	4.8 kcal/mol

Next, we extended the model to include more complex PSA cycle steps such as multiple pressure equalizations (up to 4), product pressurization, co-current depressurization to recover more of the synthesis gas trapped in the pores of the sorbent. This more complicated cycle sequence decreased the working capacity of the sorbent. However, the H_2 recovery increased

Figure 35. Simulation results showing steady state.

Figure 36. H_2 wave fronts during feed step.

providing high purity CO₂ during desorption eliminating or simplifying the need for downstream purification of the CO₂ stream before pressurization to 2,200 psig for transport and storage. The high recovery and subsequent combustion of H₂ in the gas turbine also increases the overall cycle efficiency.

In the case of low rank coals such as sub-bituminous and lignite coal there is excess water in the synthesis gas (1.94 and 3.12 steam to CO ratio, respectively). Hence the benefit of reduced steam consumption from combining the WGS and CO₂ capture would not be realized in the case of low rank coals.

Sub-bituminous Coal:

Simplified block diagram for sub-bituminous coal illustrating the integration of the 1st stage WGS with TDA's combined last stage WGS and CO₂ removal unit is shown in Figure 37. 96.4% CO conversion shown is the total conversion of CO present in the un-shifted syngas (as obtained in the field trials at steam to CO ratio of 1.1), of this 81.5% conversion takes place in the 1st stage WGS located upstream of TDA's system.

Simplified block diagram of TDA's combined WGS/warm gas CO₂ removal unit (a high temperature PSA system) for sub-bituminous coal operating on an improved 8-bed PSA cycle scheme with multiple pressure equalizations and recycle is shown in Figure 38. TDA provided the composition, pressure, and temperature of these streams (Table 10) along with the bed sizing factor for sizing the sorbent requirement (181.97 kg sorbent/kmol CO₂ in product per h) to UCI for integration with the Aspen model. UCI then completed the Aspen model and calculated the net plant efficiency for a sub-bituminous coal based IGCC plant integrated with both Selexol based cold gas CO₂ capture and TDA's combined WGS and PSA process based warm gas CO₂ capture.

Figure 37. Simplified block diagram illustrating the integration of the 1st stage WGS with TDA's combined last stage WGS and CO₂ removal unit for sub-bituminous coal.

We calculated the amount of sorbent needed as 1,888 tonnes. Table 11 summarizes the bed sizing information for the combined WGS and CO₂ capture beds for sub-bituminous coal. We designed the sorbent beds to have a L/D of 4 with three trains of 8-bed PSA systems containing a total of 24 beds that go through the PSA cycle sequence shown in Figure 39.

Table 9. System performance under optimum cycle parameters for simplified 4-step PSA cycle

H ₂ Purity (%)	99.23942
H ₂ recovery (%)	69.06249
kmol H ₂ /kg sorbent/hr	0.012244
CO ₂ purity (%)	60.1531
CO ₂ recovery (%)	98.66
kmol CO ₂ /kg sorbent/hr	0.00828
Working capacity (% wt. CO ₂) - Based on High Pressure H ₂ produced	4.985%
Working capacity (% wt. CO ₂) - Based on Low Pressure CO ₂ produced	7.286%

Note: Stream No. (5) is not used to be consistent with earlier design sheets where (5) was used for CO₂ pu stream

Figure 38. Simplified block diagram of TDA's combined WGS and CO₂ removal unit, a high temperatures PSA system for sub-bituminous coal.

Table 10. Stream summary data for TDA's combined WGS and CO₂ removal unit operating at 225°C for a Phillips 66 (E-Gas™) gasifier on sub-bituminous coal feed.

Case 2	2nd WGS in PSA beds - Sub-Bituminous Coal							
Combined 2nd WGS & CO2 removal Bed Sizing Information			Scaling Factors for Design					
Sorbent needed	1,938,798 kg		169.31 kg Sorbent/kmol CO2/h					
	4,616,185 L		23.38 L Catalyst/kmol CO/h					
Catalyst needed	27,310 L		91.3% carbon capture					
	0.6%		9305.8 Recycle compressor, kW					
Combined Sorbent & Catalyst vol.	4,643,495 L		12905.3 heat that is rejected from the PSA beds, kW					
3-trains of 8-bed each of vol.	193,479 L		44.1 heat that is rejected from the PSA beds, mmbtu/hr					
Stream No.	(1)	(2)	(3)	(4)	(6)	(7)	(8)	(9)
Description	Syngas Inlet	Steam Purge Inlet	Syngas Product	CO2 Product	Cocurrent depress out	Recycle compressor	Recycle	Bed Inlet
T (oC)	210	207.4	208.00	180.21	227.7	433	210	210
P (psia)	649.2	145.1	649.2	145.1	146.6	649.2	649.2	649.2
Flow rate (kmol/hr)	33,972	13,397	26,265	21,104	3,398	3,398	3,398	37,370
H2 (kmol/hr)	12,863		13,737	294	760	760	760	13,623
CO2 (kmol/hr)	10,581		298	11,451	2,194	2,194	2,194	12,775
H2O (kmol/hr)	8,161	13,397	11,056	9,334	379	379	379	8,540
CO (kmol/hr)	1,477		303	6	17	17	17	1,494
N2 (kmol/hr)	182		178	4	10	10	10	192
Ar (kmol/hr)	199		195	4	11	11	11	210
CH4 (kmol/hr)	503		493	11	27	27	27	530
H2S (kmol/hr)	0		0	0	0	0	0	0
NH3 (kmol/hr)	6		6	0	0	0	0	6

Table 11. TDA's Combined WGS and Warm gas CO₂ removal unit (high temperature PSA system) bed sizing summary for sub-bituminous coal.

Combined WGS & CO ₂ Capture Bed Sizing		Reactor Info	
Syngas Flowrate (fully loaded GTs), kmol/hr	33,898	Number of Trains of 8-Beds Each	3
Catalyst & Sorbent Properties		Total No. of Reactors	24
Catalyst Needed, L/(kmol CO converted/hr)	23.38	Reactor (Bed) Volume, ft ³	6,649
Sorbent Needed, kg/(kmol CO ₂ in product/hr)	169.31	Volume occupied by internal cooling tubes, ft ³	250
Sorbent bulk density, kg/L	0.42	Total Reactor Volume, ft ³	6,899
Sorbent Bulk density, lb/ft ³	26.22	Reactor Size	
CO converted in the PSA beds, kmol/hr	1,016	Aspect Ratio (Length/Diameter)	4
CO ₂ in Product, kmol/hr	11,150	Diameter, ft	13
Total Catalyst Needed, L	23,747	Length (T/T), ft	52
Total Sorbent Needed, kg	1,887,779	Reactor Volume including cooling tubes, ft ³	6,902
Total Sorbent Needed, lb	4,153,113	Operating Tempertaure, C	210
Total Sorbent Volume, L	4,494,711	Operating Pressure, bar	44.2
Total Combined catalyst & Sorbent Volume, L	4,518,458	Design Temperature, C	250
Total Combined catalyst & Sorbent Volume, ft ³	159,568	Design Pressure, bar	50

	Stage 1				Stage 2				Stage 3				Stage 4				Stage 5				Stage 6				Stage 7				Stage 8				
Time (min)	2				1	0.5	0.5	0.5	0.5	1	0.5	0.5	1	2				0.5	1.5			0.5	0.5	1	1	0.5	0.5	1	0.5	0.5			
Bed 1	ADS				EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD			PURGE				PURGE	EQ4R			EQ3R	EQ2R			EQ1R	PRESS			
Bed 2	EQ1R	PRESS			ADS				EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD			PURGE				PURGE	EQ4R			EQ3R	EQ2R			
Bed 3	EQ3R	EQ2R			EQ1R	PRESS			ADS				EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD			PURGE				PURGE	EQ4R			
Bed 4	PURGE				EQ4R	EQ3R			EQ2R	EQ1R	PRESS			ADS				EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD			PURGE			
Bed 5	PURGE				PURGE				EQ4R	EQ3R	EQ2R			EQ1R	PRESS			ADS				EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD		
Bed 6	CoDEP	BD			PURGE				EQ4R	PURGE	EQ4R			EQ3R	EQ2R			EQ1R	PRESS			ADS				EQ1D	EQ2D			EQ3D	EQ4D		
Bed 7	EQ3D	EQ4D			CoDEP	BD			PURGE				PURGE				EQ4R	EQ3R	EQ2R			EQ1R	PRESS			ADS				EQ1D	EQ2D		
Bed 8	EQ1D	EQ2D			EQ3D	EQ4D			CoDEP	BD			PURGE				PURGE				EQ4R	EQ3R	EQ2R			EQ1R	PRESS			ADS			
8- bed PSA with 4 PE and codepressurization Cycle Steps														Step 7				Blowdown to 10 bar (BD)															
Step 1	Adsorption at 44.16 bar (ADS)														Step 8				Steam Purge at 10 bar (PURGE)														
Step 2	Pressure Equalization to 36.4 bar (EQ1D)														Step 9				Pressure Equalization to 15.7 bar (EQ4R)														
Step 3	Pressure Equalization to 30.0 bar (EQ2D)														Step 10				Pressure Equalization to 23.2 bar (EQ3R)														
Step 4	Pressure Equalization to 23.2 bar (EQ3D)														Step 11				Pressure Equalization to 30.0 bar (EQ2R)														
Step 5	Pressure Equalization to 15.7 bar (EQ4D)														Step 12				Pressure Equalization to 36.4 bar (EQ1R)														
Step 6	Co-current Depressurization to 10.1 bar (CoDEP)														Step 13				Product Pressurization to 44.16 bar (PRESS)														

Figure 39. 8-bed PSA cycle scheme used for combined WGS and CO₂ capture.

Figure 40 shows a 3-D layout of the three-train of 8-bed combined WGS and PSA units with the PSA beds laid down in horizontal orientation (internal cooling tubes and connections are not shown). The selected design (i.e., horizontal orientation) will allow us to use smaller diameter reactors which ensures lower costs and easy transportation of the reactors to the application site (i.e., 13 ft reactors can be transported by rail and also can be trucked). Further design options were also considered with multiple inlets and outlets per bed to distribute the flow evenly.

Figure 40. 3-D layout of TDA's combined WGS and warm gas CO₂ removal unit in horizontal orientation (three trains of 8-bed high temperature PSA system) operating on a PSA cycle sequence with four equalizations and co-current depressurization for Sub-bituminous coal feed.

Lignite Coal:

Simplified block diagram for lignite coal illustrating the integration of the 1st stage WGS with TDA's combined last stage WGS and CO₂ removal unit is shown in Figure 41. 96.4% CO conversion shown is the total conversion of CO present in the un-shifted syngas (as obtained in the field trials at steam to CO ratio of 1.1), of this 87.1% conversion takes place in the 1st stage WGS located upstream of TDA's system.

Simplified block diagram of TDA's combined WGS/warm gas CO₂ removal unit (a high temperature PSA system) for lignite operating on an improved 8-bed PSA cycle scheme with multiple pressure equalizations and recycle is shown in Figure 42. TDA provided the composition, pressure, and temperature of these streams (Table 12) along with the bed sizing factor for sizing the sorbent requirement (181.97 kg sorbent/kmol CO₂ in product per h) to UCI for integration with the Aspen model. UCI then completed the Aspen model and calculated the net plant efficiency for a sub-bituminous coal based IGCC plant integrated with both Selexol based cold gas CO₂ capture and TDA's combined WGS and PSA process based warm gas CO₂ capture.

Figure 41. Simplified block diagram illustrating the integration of the 1st stage WGS with TDA's combined last stage WGS and CO₂ removal unit for lignite coal.

We calculated the amount of sorbent needed as 2,427 tonnes. Table 13 summarizes the bed sizing information for the combined WGS and CO₂ capture beds for sub-bituminous coal. We designed the sorbent beds to have a L/D of 5.1 with three trains of 8-bed PSA systems containing a total of 24 beds that go through the PSA cycle sequence shown in Figure 39.

Note: Stream No. (5) is not used, so as to be consistent with earlier design sheets where (5) was used for CO₂ purge stream

Figure 42. Simplified block diagram of TDA's combined WGS and CO₂ removal unit, a high temperatures PSA system for lignite coal.

Table 12. Stream summary data for TDA's combined WGS and CO₂ removal unit operating at 225°C for a Phillips 66 (E-GasTM) gasifier on lignite coal feed.

Case 3 2nd WGS in PSA beds - Lignite Coal			Scaling Factors for Design					
Combined 2nd WGS & CO ₂ removal Bed Sizing Information								
Sorbent needed	2,502,210 kg		181.97 kg Sorbent/kmol CO ₂ /h					
	5,957,644 L		28.63 L Catalyst/kmol CO/h					
Catalyst needed	17,094 L		91.1% carbon capture					
	0.3%		12010.7 Recycle compressor, kW					
Combined Sorbent & Catalyst vol.	5,974,738 L		6597.7 heat that is rejected from the PSA beds, kW					
3-trains of 8-bed each of vol.	248,947 L		22.5 heat that is rejected from the PSA beds, mmbtu/hr					
Stream No.	(1)	(2)	(3)	(4)	(6)	(7)	(8)	(9)
Description	Syngas Inlet	Steam Purge Inlet	Syngas Product	CO ₂ Product	Cocurrent depress out	Recycle compressor	Recycle	Bed Inlet
T (oC)	225	220.0	220.6	200.5	227.0	432	225	225
P (psia)	649.152	145.1	649.152	145.1	146.6	649.152	649.152	649.152
Flow rate (kmol/hr)	44,910	16,850	35,913	25,848	4,392	4,392	4,392	49,302
H ₂ (kmol/hr)	14,129		14,466	260	861	861	861	14,990
CO ₂ (kmol/hr)	13,670		516	13,751	2,601	2,601	2,601	16,270
H ₂ O (kmol/hr)	15,143	16,850	19,583	11,813	850	850	850	15,993
CO (kmol/hr)	827		226	4	13	13	13	841
N ₂ (kmol/hr)	244		240	4	14	14	14	258
Ar (kmol/hr)	272		268	5	16	16	16	288
CH ₄ (kmol/hr)	614		603	11	36	36	36	650
H ₂ S (kmol/hr)	0		0	0	0	0	0	0
NH ₃ (kmol/hr)	11		10	0	1	1	1	11

Figure 43 shows a 3-D layout of the three-train of 8-bed combined WGS and PSA units with the PSA beds laid down in horizontal orientation (internal cooling tubes and connections are not shown). The selected design (i.e., horizontal orientation) will allow us to use smaller diameter reactors which ensures lower costs and easy transportation of the reactors to the application site (i.e., 13 ft reactors can be transported by rail and also can be trucked). Further design options were also considered with multiple inlets and outlets per bed to distribute the flow evenly.

Table 13. TDA's Warm gas CO₂ removal unit (high temperature PSA system) bed sizing summary for lignite coal.

Combined WGS & CO ₂ Capture Bed Sizing		Reactor Info	
Syngas Flowrate (fully loaded GTs), kmol/hr	44,348	Number of Trains of 8-Beds Each	3
Catalyst & Sorbent Properties		Total No. of Reactors	24
Catalyst Needed, L/(kmol CO converted/hr)	28.63	Reactor (Bed) Volume, ft ³	8,526
Sorbent Needed, kg/(kmol CO ₂ in product/hr)	181.97	Volume occupied by internal cooling tubes, ft ³	250
Sorbent bulk density, kg/L	0.42	Total Reactor Volume, ft ³	8,776
Sorbent Bulk density, lb/ft ³	26.22	Reactor Size	
CO converted in the PSA beds, kmol/hr	552	Aspect Ratio (Length/Diameter)	5.1
CO ₂ in Product, kmol/hr	13,337	Diameter, ft	13
Total Catalyst Needed, L	15,805	Length (T/T), ft	66.3
Total Sorbent Needed, kg	2,426,879	Reactor Volume including cooling tubes, ft ³	8,800
Total Sorbent Needed, lb	5,339,135	Operating Tempertaure, C	232
Total Sorbent Volume, L	5,778,284	Operating Pressure, bar	44.2
Total Combined catalyst & Sorbent Volume, L	5,794,090	Design Temperature, C	270
Total Combined catalyst & Sorbent Volume, ft ³	204,616	Design Pressure, bar	50

Figure 43. 3-D layout of TDA's combined WGS and warm gas CO₂ removal unit in horizontal orientation (three trains of 8-bed high temperature PSA system) operating on a PSA cycle sequence with four equalizations and co-current depressurization for lignite coal feed.

3.6.2 Task 4.2 E-Gas™ Gasifier Performance Data for Low Rank Coals

Phillips 66 (previously known as ConocoPhillips) carried out detailed modeling of their E-GAS™ gasifier operating on two types of low rank coals, i.e., sub-bituminous and lignite and provided TDA with E-Gas™ performance data for use in the Aspen model developed in this project by UCI. The low-rank coals tend to have higher concentrations of moisture and CO₂ in the raw syngas. TDA provided Phillips 66 with two coal specifications and a required coal feed rate to be used as a basis for this Phillips 66 study. The two cases are described in Table 14. The feedstock specifications and design basis used by Phillips 66 are provided in Table 15 and Table 16. Phillips 66 provided TDA and UCI with the gasifier performance results and block flow diagrams with stream summaries around the gasifier for the two cases. Table 17 shows the summary of the E-Gas™ gasifier performance on the two low rank coals.

Table 14. Case descriptions for the E-Gas™ gasifier performance study by Phillips 66.

Case No.	Case Description	Feedstock	Basis	Syngas Production Capacity	Number of Trains
1	Montana Rosebud PRB	Sub-bituminous Coal	Nominal coal feed rate of 675,000 lb/hr (as received)	290 MMscfd CO + H ₂	3
2	North Dakota Beulah-Zap Lignite	Lignite Coal	Nominal coal feed rate of 675,000 lb/hr (as received)	197 MMscfd CO + H ₂	3

Table 15. Coal specification used by Phillips 66. Source: DE-FOA0000496.

Selected Feedstock			Case 1: Sub-bituminous	Case 2: Lignite
Equilibrium Moisture	Estimated	%	23.19	32.47
Total Moisture (as rec'd)		%	25.77	36.08
Proximate Analysis (Dry Basis)	Volatile Matter	%	40.87	41.49
	Ash	%	11.04	15.43
	Fixed Carbon	%	48.09	48.09
Hardgrove Grindability Index	HGI		57	
Heating Value (Dry Basis)	(HHV)	Btu/lb	11,516	10,427
Ultimate Analysis (Dry Basis)	C	%	67.45	61.88
	H	%	4.56	4.29
	N	%	0.96	0.98
	S	%	0.98	0.98
	O	%	15.01	16.44
	Ash	%	11.03	15.43
	Cl	%	0.01	0.00
Ash Analysis (Dry Basis)	SiO ₂	%	38.09	35.06
	Al ₂ O ₃	%	16.73	12.29
	Fe ₂ O ₃	%	6.46	5.12
	CaO	%	16.56	14.39
	MgO	%	4.25	6.61
	Na ₂ O	%	0.54	5.18
	K ₂ O	%	0.38	0.64
	TiO ₂	%	0.72	0.58
	MnO ₂ / Mn ₃ O ₄	%	-	-
	SO ₃	%	15.08	16.27
	P ₂ O ₅	%	0.35	0.56
	BaO	%	0.00	0.27
	SrO	%	0.00	0.02
	ZnO	%	-	-

Table 16. Design basis used to determine gasifier performance.

Parameter Value Units	Value	Units
Coal Flow Rate (as-received basis)	675,000	lb/hr
Oxygen purity	95	%
Boiler Feed Water Temperature	612	F
HP Steam Pressure	1950	psia
Gasifier Pressure	735	psia
Methane Content	<5%	of C

Table 17. E-Gas™ gasifier performance provided by Phillips 66.

Parameter	Case 1	Case 2	Units
Slurry Concentration	53.8	47.3	wt. %
O ₂ : Coal Ratio	0.81	0.86	lb O ₂ : lb Coal (dry)
Overall Carbon Conversion	99.1	98.7	%
Gasifier Pressure	735	735	psia

3.6.3 Task 4.2 Process Design and Aspen Model Development

Figure 44. IGCC Plant Integrated with TDA's Combined Shift and Regenerable Sorbent CO₂ Capture Process.

Figure 44 shows a simplified block diagram of an IGCC plant integrated with TDA's combined shift and high temperature PSA-based CO₂ capture / purification process (blocks in green). TDA's Warm Gas CO₂ capture system is located downstream of a warm gas desulfurization system (we used the regenerable zinc-titanate-based syngas desulfurization system developed by the Research Triangle Institute). The regeneration off-gas from the desulfurization system is further treated in a sulfuric acid plant, ultimately converting all sulfur into a concentrated H₂SO₄ byproduct. The desulfurized synthesis gas is then fed to a first adiabatic shift reactor for the (partial) conversion of the CO into H₂. The synthesis gas from the first shift unit after heat recovery is then sent to the combined shift and CO₂ capture system at a temperature (at least 30°C) above the dew point of the syngas. The decarbonized syngas leaves this system with a significant amount of moisture in it and is fed to the gas turbines after preheating to maximize overall plant efficiency. The TDA's Warm Gas cleanup process thus eliminates the need to cool the synthesis gas below its dew point using condensing heat exchangers.

The CO₂ purification/compression system further treats the CO₂ stream from the separation unit into a high purity, pressurized CO₂ byproduct that meets pipeline specifications. Any gases trapped in the voids of the sorbent and the reactor ullage space are recovered at an intermediate pressure and recycled back to the syngas feed to ensure high H₂ recovery in the CO₂ separation unit. A steam purge at lower pressure is used to fully regenerate the sorbent. A CO₂ rich stream primarily consisting of H₂O and CO₂ (along with some CO and H₂ impurities) is sent for further purification consisting of a catalytic combustor to burn any residual syngas with oxygen) and compression, liquefaction and pumping to produce a high purity CO₂ stream at 15.3 MPa (2,215 psia) that can be sent for sequestration.

Process Design Basis and Methodology

Consistency has been maintained between the IGCC case developed under this study utilizing the TDA's high temperature PSA-based CO₂ capture process (**Warm Gas Cleanup Cases**) with the Phillips 66 gasifier based IGCC plant with CO₂ capture utilizing current state-of-the-art syngas cleanup and CO₂ capture technology (**Cold Gas Cleanup Cases**).

The combined shifting and CO₂ adsorption in the Warm Gas Cleanup cases uses a shift catalyst along with TDA's low cost, high capacity CO₂ sorbent in the same vessel equipped with internal heat transfer tubes generating steam while maintaining near isothermal bed conditions. The sorbent can also simultaneously remove the trace contaminants such as Hg and As that are present in the synthesis gas. Performance data for the shifting and CO₂ adsorption unit (with co-sorption of Hg) were provided by TDA and consisted of the definition of the streams (composition, flow rate, temperature and pressure) associated with this subsystem for a partially shifted syngas stream (leaving the 1st shift reactor operated under adiabatic conditions) as estimated by UCI. Sizing basis for the combined shifting and CO₂ sorption vessels using the pressure swing adsorption (PSA) process was also provided by TDA.

Site Conditions: The plants are designed for the following mean ambient conditions which are the same as those in the previous DOE/NETL study (DOE/NETL-2010/1399):

Montana Site Ambient Conditions for PRB Coal Cases:

- Elevation, m (ft) = 1,036 (3,400)
- Barometric Pressure, MPa (psia) = 0.09 (13.0)
- Design Ambient Temperature, Dry Bulb, °C (°F) = 5.6 (42)
- Design Ambient Temperature, Wet Bulb, °C (°F) = 2.8 (37)
- Design Ambient Relative Humidity, % = 62

North Dakota Site Ambient Conditions for Lignite Coal Cases:

- Elevation, m (ft) = 579 (1,900)
- Barometric Pressure, MPa (psia) = 0.10 (13.8)
- Design Ambient Temperature, Dry Bulb, °C (°F) = 4.4 (40)
- Design Ambient Temperature, Wet Bulb, °C (°F) = 2.2 (36)
- Design Ambient Relative Humidity, % = 68

A parallel wet/dry condenser was chosen for all plant configurations since these plants are located in the Western U.S. and need to consider limited water supplies which is consistent with the previous DOE/NETL study (DOE/NETL-2010/1399). In this parallel cooling system, half of the turbine exhaust steam is condensed in an air-cooled condenser and the remaining half in a water-cooled condenser. The cooling water is provided by a mechanical draft, evaporative cooling tower.

The site characteristics are assumed to be the same for both plant locations which are the same as in the previous DOE/NETL study (DOE/NETL-2010/1399):

- Location: Greenfield
- Topography: Level
- Size, acres: 300
- Transportation: Rail
- Ash/Slag Disposal: Off Site

- Makeup Water: Municipal (50%) / Groundwater (50%)
- Access: Landlocked, having access by rail and highway
- CO₂ Storage: Compressed to 15.3 MPa (2,215 psia), transported 80 kilometers (50 miles) and sequestered in a saline formation at a depth of 1,239 meters (4,055 feet)

It is assumed that the land area required for all cases is 30 acres for the plant proper, and the balance provides a buffer of approximately 0.25 miles to the fence line. The extra land could also provide for a rail loop if required. In all cases it is assumed that the steam turbine is enclosed in a turbine building, but the gasifiers are not enclosed. The following design parameters are not quantified for this study as these are considered site-specific, and allowances only for normal conditions and construction are included in the cost estimates.

- Flood plain considerations
- Existing soil/site conditions
- Water discharges and reuse
- Rainfall/snowfall criteria
- Seismic design
- Buildings/enclosures
- Fire protection
- Local code height requirements
- Noise regulations – Impact on site and surrounding area

Coal Feed: The characteristics of the coal feed are the same as that in the previous DOE/NETL study (DOE/NETL-2010/1399) and are shown in Table 18 and Table 19.

Carbon Dioxide Product Specification:

The specifications of the CO₂ product are based on the typical purity obtained by the Selexol™ cold gas cleanup process which was used in the previously referenced DOE/NETL report without any further purification. The Argon content in the CO₂ stream coming off the TDA's PSA unit is similar to what is typically obtained from a Selexol™ unit, i.e., without any further purification. This eliminated the need for cryogenic distillation in the CO₂ purification process and instead a catalytic combustor to burn any residual syngas present in the CO₂ stream with oxygen from the air separation unit (ASU) was utilized. Table 20 summarizes the CO₂ specifications used for this analysis.

Table 18. Montana Rosebud PRB, Area D, Western Energy Co. Mine, Subbituminous Design Coal Analysis.

	Subbituminous	
Proximate Analysis	Dry Basis, %	As Received, %
Moisture	0	25.77
Ash	11.04	8.19
Volatile Matter	40.87	30.34
Fixed Carbon	48.09	35.7
Total	100	100
Ultimate Analysis	Dry Basis, %	As Received, %
Carbon	67.45	50.07
Hydrogen	4.56	3.38
Nitrogen	0.96	0.71
Sulfur	0.98	0.73
Chlorine	0.01	0.01
Ash	11.03	8.19
Moisture	0	25.77
Oxygen	15.01	11.14
Total	100	100
Heating Value	Dry Basis	As Received
HHV, kJ/kg	26,787	19,920
HHV, Btu/lb	11,516	8,564
LHV, kJ/kg	25,810	19,195
LHV, Btu/lb	11,096	8,252
Trace Components		
Mercury ^[1] , ppm		0.081

^[1]Mercury content is the mean plus one standard deviation using EPA's ICR data.

Table 19. North Dakota Beulah-Zap Lignite, Freedom, ND Mine, Lignite Design Coal Analysis.

	Lignite	
Proximate Analysis	Dry Basis, %	As Received, %
Moisture	0	36.08
Ash	15.43	9.86
Volatile Matter	41.49	26.52
Fixed Carbon	43.09	27.54
Total	100	100
Ultimate Analysis	Dry Basis, %	As Received, %
Carbon	61.88	39.55
Hydrogen	4.29	2.74
Nitrogen	0.98	0.63
Sulfur	0.98	0.63
Chlorine ^[2]	18 ppmw	12 ppmw
Ash	15.43	9.86
Moisture	0	36.08
Oxygen	16.44	10.51
Total	100	100
Heating Value	Dry Basis	As Received
HHV, kJ/kg	24,253	15,391
HHV, Btu/lb	10,427	6,617
LHV, kJ/kg	23,334	14,803
LHV, Btu/lb	10,032	6,364
Trace Components		
Mercury, ppm		0.116

^[2] The Cl content is taken from paper titled, "Comparison of Sorbents and Furnace Additives for Mercury Control in Low Rank Fuel Combustion Systems," by C. R. Crocker, S. A. Benson, M. J. J. Holmes, Y. Zhuang, J. H. Pavlish, K. C. Galbreath [Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem. 2004, 49 (1), 289]

Table 20. CO₂ Pipeline Specification.

Parameter Units	Parameter Value
Inlet Pressure MPa (psia)	15.3 (2,215)
Outlet Pressure MPa (psia)	10.4 (1,515)
Inlet Temperature °C (°F)	35 (95)
CO ₂ Concentration, mole %	> 95
N ₂ Concentration	not limited
O ₂ Concentration ppmv	< 40
Ar Concentration	not limited
H ₂ O Concentration ppmv	< 150

Property Packages: The performance of the plant was estimated using the Aspen Plus Simulator software, and the following property packages were used to model the cycle:

- PR-BM (Peng-Robinson equation of state with Boston-Mathias modifications) for most plant section systems except as follows
- ElecNRTL (Electrolyte Non-random Two Liquid model, also known as the Chen electrolyte model, formulated for modeling aqueous electrolytes) for sour water systems
- STEAM-TA (ASME 1967 Steam Table Corrections) for the water and steam.

Process Descriptions

Cold Gas Cleanup: The IGCC plant employing the cold gas cleanup and CO₂ capture technology depicted in Figure 3-1 consists of the following plant subsystems. The major stream data for the subbituminous and the lignite are presented in Tables 3-1 and 3-2 for a coal feed rate of 292,295 kg/h on an “as received” basis. Note that this flow rate of coal does not fully load the two gas turbines and the corresponding stream data should be scaled to fully load the two gas turbines. This coal flow rate however is held the same as in the corresponding Warm Gas Cleanup cases and allows a more direct comparison of the various plant streams between the two subbituminous cases and between the two lignite cases (but not for cross comparison between the two different types of coals).

- Air Separation Unit (ASU)
- Coal Feed Preparation
- Gasification (based on Phillips 66 technology)
- High Temperature Syngas Cooling and Scrubbing
- Sour Shifting and Cold Gas Heat Recovery
- Syngas Desulfurization and Decarbonization using a two-stage Selexol™ process
- Claus Sulfur Recovery and Tail Gas Hydrogenation followed by Recycle to the Gasifier
- CO₂ Dehydration and Pressurization (the pressurization scheme was modified to include first compression to a pressure such that the CO₂ stream forms a liquid when cooled against the cooling water, followed by pumping to the final pressure in order to reduce the parasitic load of pressurization)
- Gas Turbine (based on GE F class technology type)
- Heat Recovery Steam Generator Unit
- Reheat Steam Cycle

The plant also has the necessary utilities (e.g. cooling water supply, make-up water treatment, plant and instrument air) to support the process units. Detailed process description of this type of plant may be found in the previously referenced DOE/NETL report.

Warm Gas Cleanup: The IGCC plant employing the sorbent CO₂ capture consists of the following plant subsystems:

- Air Separation Unit (ASU)
- Coal Feed Preparation
- Gasification (based on Phillips 66 technology)
- High Temperature Syngas Cooling and Scrubbing
- Warm Gas Cleanup similar to RTI's process including Acid (H₂SO₄) Unit
- First Stage of Shifting

- Combined Shifting and Regenerable Sorbent CO₂ Capture (based on TDA technology)
- CO₂ Purification and Pressurization
- Gas Turbine (based on GE F class technology type)
- Heat Recovery Steam Generator Unit
- Reheat Steam Cycle

The overall configuration of the IGCC plant with TDA's combined shift and high temperature PSA-based CO₂ capture system is shown in Figure 3-2 while the major stream data for the subbituminous and the lignite cases are presented in Tables 3-3 and 3-4. Plant subsystems that are different from the Cold Gas Cleanup case are described in the following.

As in the cold gas cleanup case, 7% of the raw syngas exiting the scrubber is compressed and recycled back to the gasifier system as quench gas.

Remainder of the scrubbed gas is preheated to a temperature of 260°C in a feed/effluent exchanger and supplied to a warm gas cleanup unit similar to RTI's process for removal of sulfur compounds utilizing a zinc titanate adsorbent in a fluidized bed. The performance of this unit as well as the production of H₂SO₄ from the SO₂ in the regenerator off-gas was developed utilizing information available in the public domain. The regenerator off-gas after particulate removal is depressurized by expansion in a power recovery turbine before feeding it to the H₂SO₄ unit. The on-site ASU provides the small amount of O₂ as required by the H₂SO₄ unit in addition to supplying oxygen to the gasifier and the catalytic combustor used for CO₂ purification (combust the residuals amounts of H₂, CO and CH₄). The hot syngas leaving the desulfurizer is cooled (to a temperature of 224°C for the subbituminous case and 231°C for the lignite case) in the feed/effluent exchanger where the desulfurizer feed gas is preheated.

The clean gas is then treated in a shift reactor similar to the 1st stage reactor of the Cold Gas Cleanup case. The effluent is cooled by generating intermediate pressure (IP) and medium pressure (MP) steam. The partially shifted syngas leaving this shift reactor (at a temperature of 210°C for the subbituminous case and 232°C for the lignite case) is combined with recycle gas from the downstream TDA's combined shift and PSA unit and then fed to this TDA's unit for further shifting and simultaneously decarbonizing the syngas before it is combusted in the gas turbines as depicted in Figure 3-3. About 98% of the syngas enters this simultaneous shifting and decarbonizing unit to result in an overall carbon capture of 90%. Remainder of the syngas is sent directly to the gas turbine bypassing TDA's CO₂ capture system. Regeneration is accomplished utilizing steam at a desorption pressure of 10 barA. Two streams are regenerated, one consisting of "raw CO₂," a mixture of CO₂, steam and small amounts of residual syngas at the desorption pressure and the other "recycle gas," with significant amounts of other syngas components (mainly H₂) at a lower pressure of 9.38 bar for recycle to the combined shift and CO₂ separation unit. The raw CO₂ is cooled in a series of heat exchangers while generating low pressure (LP) steam, vacuum condensate/makeup BFW heating and finally trim cooled against cooling water before it is compressed, preheated in a feed/effluent exchanger and then fed to a catalytic (noble meta containing) combustor along with O₂ to oxidize the small amounts of combustibles present in the raw CO₂ stream. The effluent from this combustor after generating HP steam is cooled in the feed/effluent exchanger. This is followed by vacuum condensate/makeup BFW heating and finally trim cooled against cooling water. It is then further compressed to a pressure such that the CO₂ stream forms a liquid when cooled against the cooling water. This liquid CO₂ stream leaving the cooling water exchanger is

then pumped to the final pressure (note that a similar scheme was used in the Cold Gas Cleanup case to maintain consistency).

The decarbonized syngas leaving the combined shift and CO₂ separation (adsorption) unit (at a temperature of 208°C in the case of the subbituminous coal and 221°C in the case of the lignite) with its accompanying unreacted steam is supplied to the gas turbines. In the case of the subbituminous coal, additional diluent in the form of N₂ (pressurized, humidified and preheated) from the ASU is required, the amount of N₂ added is significantly lower than that in the corresponding Cold Gas Cleanup case due to the large amount of water vapor present in the syngas. The combined cycle design is similar to the design in the Cold Gas Cleanup case consisting of a reheat steam cycle.

Figure 45. Block flow diagram for IGCC plant with cold gas CO₂ capture system.

Figure 46. Block flow diagram for IGCC plant with TDA’s combined shift and high-temperature PSA-based CO₂ capture system.

Figure 47. Block flow diagram of TDA's combined shift and high temperature PSA-based CO₂ capture system along with the CO₂ purification and compression system.

Table 21. Stream Data: Cold Gas Cleanup – Lignite Coal (292,295 kg/h as received).

STREAM NO.	1	2	3	4	5	6	7	8	9	9A	10	11	12
Temperature, C	15	91	149	79	232	218	58	60	206	398	38	345	226
Pressure, bar	1.01	59.64	66.19	70.67	7.93	30.52	3.1	1.01	48.72	51.02	43.89	7.31	2.1
Solids, kg/hr	292345	0	292345	0	0	0	5587	19666	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	0.001	0	1	1	1	1	1
kmol/hr (w/o Solids)	0	0.01	6162	5917	52	15975	353	0	35334	1566	26008	3013	386
kg/hr (w/o Solids)	0	0.292	111015	190420	1673	448307	6373	0	730087	28216	555517	54273	14140
Mole Frac (w/o Solids)													
O ₂	0	0.005	0	0.95	0.95	0.005	0	0	0	0	0	0	0
N ₂	0	0.992	0	0.018	0.018	0.992	0	0	0.005	0	0.007	0	0.001
Ar	0	0.002	0	0.032	0.032	0.002	0	0	0.006	0	0.007	0	0.002
H ₂	0	0	0	0	0	0	0	0	0.213	0	0.518	0	0.112
CO	0	0	0	0	0	0	0	0	0.206	0	0.012	0	0.004
CO ₂	0	0	0	0	0	0	0	0	0.146	0	0.434	0	0.675
H ₂ O	0	0	1	0	0	0	0.998	0	0.406	1	0.001	1	0.021
CH ₄	0	0	0	0	0	0	0	0	0.015	0	0.019	0	0.01
H ₂ S	0	0	0	0	0	0	0	0	0.002	0	0.003	0	0.175
HCl	0	0	0	0	0	0	0.002	0	0	0	0	0	0

STREAM NO.	13	14	15	16	17	18	19	20	21	22	23
Temperature, C	174	139	14	11	11	32	21	218	6	564	154
Pressure, bar	1.45	63.4	10.93	17.24	20.62	152.7	41.44	40.75	0.9	0.93	0.87
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	1	1	0.989	0	1	1	1	1	1
kmol/hr (w/o Solids)	33	305	5528	3938	1404	10855	15041	15041	107876	132034	132034
kg/hr (w/o Solids)	2125	11971	243306	173326	59236	475575	77258	77258	3117040	3642610	3642610
Mole Frac (w/o Solids)											
O ₂	0	0	0	0	0	0	0	0	0.208	0.112	0.112
N ₂	0	0.016	0	0	0	0	0.012	0.012	0.776	0.755	0.755
Ar	0	0.008	0	0	0.001	0	0.013	0.013	0.009	0.009	0.009
H ₂	0	0.093	0	0	0.03	0.004	0.891	0.891	0	0	0
CO	0	0.008	0	0	0.003	0	0.021	0.021	0	0	0
CO ₂	0	0.857	1	1	0.947	0.995	0.032	0.032	0	0.01	0.01
H ₂ O	0	0.004	0	0	0.012	0	0	0	0.006	0.114	0.114
CH ₄	0	0.009	0	0	0.007	0.001	0.031	0.031	0	0	0
H ₂ S	0	0.004	0	0	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0	0	0

Table 22. Stream Data: Cold Gas Cleanup – Lignite Coal (292,295 kg/h as received).

STREAM NO.	1	2	3	4	5	6	7	8	9	9A	10	11	12
Temperature, C	15	94	149	72	232	215	58	60	215	265	38	331	226
Pressure, bar	1.01	59.64	66.19	71.69	7.93	30.52	3.1	1.01	48.72	51.02	43.89	7.31	2.1
Solids, kg/hr	292345	0	292345	0	0	0	6712	23625	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	0	0	1	0.678	1	1	1
kmol/hr (w/o Solids)	0	0.01	5702	5295	47	19598	3958	0	31290	0	19225	2421	306
kg/hr (w/o Solids)	0	0.292	102722	170419	1503	549977	71314	0	662319	3	438058	43608	11397
Mole Frac (w/o Solids)													
O ₂	0	0.005	0	0.95	0.95	0.005	0	0	0	0	0	0	0
N ₂	0	0.992	0	0.018	0.018	0.992	0	0	0.005	0	0.008	0	0.001
Ar	0	0.002	0	0.032	0.032	0.002	0	0	0.006	0	0.009	0	0.003
H ₂	0	0	0	0	0	0	0	0	0.181	0	0.484	0	0.097
CO	0	0	0	0	0	0	0	0	0.143	0	0.006	0	0.002
CO ₂	0	0	0	0	0	0	0	0	0.17	0	0.468	0	0.678
H ₂ O	0	0	1	0	0	0	1	0	0.479	1	0.001	1	0.019
CH ₄	0	0	0	0	0	0	0	0	0.013	0	0.019	0	0.01
H ₂ S	0	0	0	0	0	0	0	0	0.002	0	0.003	0	0.189

STREAM NO.	13	14	15	16	17	18	19	20	21	22	23
Temperature, C	174	138	13	11	11	31	20	215	4	561	152
Pressure, bar	1.45	63.4	10.93	17.24	20.62	152.7	41.44	40.75	0.95	0.99	0.93
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	1	1	0.99	0	1	1	1	1	1
kmol/hr (w/o Solids)	29	246	4362	3109	1103	8562	10574	10574	64597	90074	90074
kg/hr (w/o Solids)	1829	9773	191983	136818	46758	375347	60627	60627	1866670	2477280	2477280
Mole Frac (w/o Solids)											
O ₂	0	0	0	0	0	0	0	0	0.208	0.09	0.09
N ₂	0	0.024	0	0	0.001	0	0.015	0.015	0.776	0.774	0.774
Ar	0	0.01	0	0	0.001	0	0.016	0.016	0.009	0.009	0.009
H ₂	0	0.081	0	0	0.026	0.003	0.877	0.877	0	0	0
CO	0	0.006	0	0	0.001	0	0.011	0.011	0	0	0
CO ₂	0	0.861	1	1	0.953	0.995	0.046	0.046	0	0.011	0.011
H ₂ O	0	0.004	0	0	0.011	0	0	0	0.006	0.115	0.115
CH ₄	0	0.009	0	0	0.007	0.001	0.034	0.034	0	0	0
H ₂ S	0	0.005	0	0	0	0	0	0	0	0	0

Table 23. Stream Data: Warm Gas Cleanup – Subbituminous Coal (292,295 kg/h as received).

STREAM NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Temperature, C	15	86	149	92	59	32	288	145	59	60	205	15	334	6	141	20	43	210
Pressure, bar	1.01	51.37	66.19	70.67	41.2	8.62	30.52	20.5	3.1	1.01	48.72	1.01	2.07	0.9	8	1.01	1.01	44.16
Solids, kg/hr	292345	0	292345	0	0	0	0	0	5587	19666	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	1	1	0.013	0	1	1	1	1	0	0	1	1
kmol/hr (w/o Solids)	0	0.01	6162	5906	108	40	5215	169	46	0	34840	506	576	201	64	66	718	32783
kg/hr (w/o Solids)	0	0.292	111015	190083	3028	1290	133873	5454	835	0	720954	14607	18612	5820	1159	6490	20419	676307
Mole Frac (w/o Solids)																		
O ₂	0	0.005	0	0.95	0.005	0.95	0.004	0.95	0	0	0	0.208	0.011	0.208	0	0	0.074	0
N ₂	0	0.992	0	0.018	0.992	0.018	0.756	0.018	0	0	0.005	0.772	0.864	0.776	0	0	0.913	0.005
Ar	0	0.002	0	0.032	0.002	0.032	0.002	0.032	0	0	0.006	0.009	0.009	0.009	0	0	0.011	0.006
H ₂	0	0	0	0	0	0	0	0	0	0	0.216	0	0	0	0	0	0	0.381
CO	0	0	0	0	0	0	0	0	0	0	0.209	0	0	0	0	0	0	0.04
CO ₂	0	0	0	0	0	0	0	0	0	0	0.148	0	0	0	0	0	0.001	0.314
H ₂ O	0	0	1	0	0	0	0.238	0	0.987	0	0.398	0.011	0.001	0.006	1	0.005	0.001	0.24
CH ₄	0	0	0	0	0	0	0	0	0	0	0.015	0	0	0	0	0	0	0.015
H ₂ S	0	0	0	0	0	0	0	0	0	0	0.002	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0.013	0	0	0	0	0	0	0	0	0
SO ₂	0	0	0	0	0	0	0	0	0	0	0	0	0.115	0	0	0	0	0
H ₂ SO ₄	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.995	0	0

STREAM NO.	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
Temperature, C	207	180	39	208	6	577	153	228	209	26	92	288	430	136	26	57	20
Pressure, bar	10.34	10	152.7	42.57	0.9	0.93	0.87	10.11	44.16	9.38	20	19.79	19.1	18.55	17.79	60	59.66
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0
kmol/hr (w/o Solids)	12591	19751	10794	25309	102387	126158	126158	3191	34944	11099	11099	11099	11128	11128	10794	10794	10794
kg/hr (w/o Solids)	226835	631332	474904	266134	2958430	3358440	3358440	100075	755949	475459	475459	475459	480913	480913	474904	474904	474904
Mole Frac (w/o Solids)																	
O ₂	0	0	0	0	0.208	0.108	0.108	0	0	0	0	0	0	0	0	0	0
N ₂	0	0	0.001	0.007	0.776	0.662	0.662	0.003	0.005	0	0	0	0.001	0.001	0.001	0.001	0.001
Ar	0	0	0.001	0.007	0.009	0.009	0.009	0.003	0.006	0	0	0	0.001	0.001	0.001	0.001	0.001
H ₂	0	0.014	0	0.521	0	0	0	0.224	0.398	0.025	0.025	0.025	0	0	0	0	0
CO	0	0	0	0.013	0	0	0	0.005	0.009	0.001	0.001	0.001	0	0	0	0	0
CO ₂	0	0.545	0.999	0.02	0	0.011	0.011	0.646	0.375	0.97	0.97	0.97	0.969	0.969	0.999	0.999	0.999
H ₂ O	1	0.44	0	0.413	0.006	0.21	0.21	0.111	0.193	0.003	0.003	0.003	0.03	0.03	0	0	0
CH ₄	0	0.001	0	0.019	0	0	0	0.008	0.014	0.001	0.001	0.001	0	0	0	0	0
H ₂ S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO ₂	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H ₂ SO ₄	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 24. Stream Data: Warm Gas Cleanup – Lignite Coal (292,295 kg/h as received).

STREAM NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Temperature, C	15	93	149	95	60	28	196	518	58	60	213	4	334	4	141	20	43	232
Pressure, bar	1.01	51.37	66.19	70.67	41.2	1.03	30.52	20.5	3.1	1.01	48.72	0.95	2.07	0.95	8	1.01	1.01	44.16
Solids, kg/hr	292345	0	292345	0	0	0	0	0	6712	23625	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	1	1	0	0	1	1	1	1	0	0	1	1
kmol/hr (w/o Solids)	0	0	5702	5283	92	34	0	100	3956	0	30318	433	494	173	55	58	619	28193
kg/hr (w/o Solids)	0	0	102722	170031	2574	1106	0	3211	71278	0	644934	12499	15946	4987	995	5602	17644	598842
Mole Frac (w/o Solids)																		
O ₂	0	0.005	0	0.95	0.005	0.95	0.005	0.95	0	0	0	0.208	0.011	0.208	0	0	0.07	0
N ₂	0	0.992	0	0.018	0.992	0.018	0.992	0.018	0	0	0.005	0.776	0.864	0.776	0	0	0.908	0.005
Ar	0	0.002	0	0.032	0.002	0.032	0.002	0.032	0	0	0.006	0.009	0.009	0.009	0	0	0.011	0.006
H ₂	0	0	0	0	0	0	0	0	0	0	0.184	0	0	0	0	0	0	0.315
CO	0	0	0	0	0	0	0	0	0	0	0.149	0	0	0	0	0	0	0.018
CO ₂	0	0	0	0	0	0	0	0	0	0	0.174	0	0	0	0	0	0.007	0.305
H ₂ O	0	0	1	0	0	0	0	0	1	0	0.465	0.006	0.001	0.006	1	0.018	0.003	0.336
CH ₄	0	0	0	0	0	0	0	0	0	0	0.014	0	0	0	0	0	0	0.014
H ₂ S	0	0	0	0	0	0	0	0	0	0	0.002	0	0	0	0	0	0	0
SO ₂	0	0	0	0	0	0	0	0	0	0	0	0	0.115	0	0	0	0	0
H ₂ SO ₄	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.982	0	0

STREAM NO.	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
Temperature, C	205	201	38	221	4	580	152	227	225	26	93	288	398	136	27	56	19
Pressure, bar	10.34	10	152.7	42.57	0.95	0.99	0.93	10.11	44.16	9.25	20	19.79	19.1	18.55	17.79	60	59.66
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0
kmol/hr (w/o Solids)	10375	15729	8487	22360	68798	86538	86538	2691	29853	8671	8671	8671	8689	8689	8487	8487	8487
kg/hr (w/o Solids)	186916	500997	373410	276106	1988050	2264150	2264150	81967	660444	373843	373843	373843	377053	377053	373410	373410	373410
Mole Frac (w/o Solids)																	
O ₂	0	0	0	0	0.208	0.103	0.103	0	0	0	0	0	0	0	0	0	0
N ₂	0	0	0.001	0.007	0.776	0.619	0.619	0.003	0.005	0	0	0	0.001	0.001	0.001	0.001	0.001
Ar	0	0	0.001	0.007	0.009	0.009	0.009	0.004	0.006	0	0	0	0.001	0.001	0.001	0.001	0.001
H ₂	0	0.01	0	0.406	0	0	0	0.197	0.322	0.018	0.018	0.018	0	0	0	0	0
CO	0	0	0	0.007	0	0	0	0.003	0.005	0	0	0	0	0	0	0	0
CO ₂	0	0.538	0.999	0.022	0	0.012	0.012	0.595	0.348	0.977	0.977	0.977	0.976	0.976	0.999	0.999	0.999
H ₂ O	1	0.451	0	0.534	0.006	0.257	0.257	0.19	0.3	0.003	0.003	0.003	0.023	0.023	0	0	0
CH ₄	0	0	0	0.017	0	0	0	0.008	0.013	0.001	0.001	0.001	0	0	0	0	0
H ₂ S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO ₂	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H ₂ SO ₄	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

3.7 Task 5. System and Process Economic Analysis

Under subcontract to TDA, the Advanced Power and Energy Program of the University of California, Irvine (UCI), provided assistance in the process design and developed system simulation models to assess the economic viability of TDA's combined shift and high temperature PSA-based pre-combustion carbon capture (Warm Gas Cleanup) technology. The analysis also provided thorough comparison against the conventional cold gas cleanup technology utilizing the Selexol™ physical solvent scrubbing (used for desulfurization and de-carbonization of the raw syngas). The gasification system performance was provided by Phillips 66 for the lignite coal from North Dakota. These data consisted of the definition of all key process parameters including the gas composition, flow rate, temperature and pressure of each process stream entering and leaving each of the gasification systems (from the incoming coal slurry and oxygen to the outgoing raw scrubbed syngas). The performance data for the combined shift and CO₂ removal system was provided by TDA that consisted again of the definition of all key process parameters including the gas composition, flow rate, temperature and pressure of each process stream entering and leaving this combined system. UCI then developed the overall process model with all sub-systems for the site specific conditions. Prior to the process design and modeling, the accuracy of the Aspen Plus® model was verified by checking the simulation results against the data provided by Phillips 66.

The plant performance of the four cases is summarized in Table 25 and Table 26 with the flow rates scaled to fully load the two gas turbines. It should be noted that the performance of the gas turbine for each of these cases was estimated by UCI and it is recommended that in a more detailed phase of this development program, gas turbine vendors be contacted for providing performance data. The effective LHV of the syngas provided to the gas turbines was held constant for each of the cases by adjusting the amount of diluent, i.e., moisture introduced into the syngas by the humidification operation in the case of cold gas cleanup, and amount of humidified nitrogen (supplied by the ASU) in the case of the subbituminous coal warm gas cleanup case while the lignite warm gas cleanup case required no additional diluent in the form of N₂. The need for the additional diluent in the form of humidified nitrogen in the subbituminous coal warm gas cleanup case limited its efficiency gain over the corresponding cold gas cleanup case. The molar ratio of moisture to N₂ is significantly higher for the warm gas cleanup case and since H₂O has a much higher specific heat than N₂, it may be expected that the NO_x emission for this case will be significantly lower. We also carried out comparison of the warm gas cleanup cases against the cold gas cleanup cases on the basis of same coal feed rate of 292,295 kg/h (as received) and the performance results are summarized in Table 27 and Table 28 for the two types of coal.

The plant cost and the levelized cost of electricity estimates for the Cold Gas Cleanup Cases and the Warm gas Cleanup Cases are presented in Table 29 through Table 32 with the flow rates scaled to fully load the two gas turbines.

Table 25. Overall Plant Performance Summary: Subbituminous Coal Cases Fully Loaded GTs.

	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	Kwe	430,900	430,900
STEAM TURBINE POWER	Kwe	262,055	254,311
TOTAL GROSS POWER	Kwe	692,955	685,211
TOTAL AUXILIARY CONSUMPTION	Kwe	181,112	134,862
NET POWER OUTPUT	Kwe	511,843	550,349
AUXILIARY LOAD SUMMARY			
COAL HANDLING	Kwe	599	614
COAL MILLING	Kwe	3,036	3,110
COAL SLURRY PUMPS	Kwe	658	674
SLAG HANDLING & DEWATERING	Kwe	1,499	1,534
AIR SEPARATION UNIT AUXILIARIES	Kwe	1,162	1,219
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	Kwe	65,733	49,412
OXYGEN COMPRESSOR	Kwe	15,579	23,681
NITROGEN COMPRESSOR	Kwe	29,941	7,984
SYNGAS RECYCLE COMPRESSOR	Kwe	520	532
TAIL GAS RECYCLE COMPRESSOR	Kwe	1,584	-
CO2 PURIFICATION & COMPRESSION	Kwe	20,345	25,499
BOILER FEEDWATER & DEMIN PUMPS	Kwe	4,459	4,891
VACUUM CONDENSATE PUMP	Kwe	283	290
PROCESS CONDENSATE & SWS SYSTEMS	Kwe	235	580
BFW CIRCULATING PUMPS	Kwe	23	97
COOLING WATER CIRCULATING PUMPS	Kwe	3,411	2,965
COOLING TOWER + AIR COOLER FANS	Kwe	5,277	4,469
SCRUBBER PUMPS	Kwe	95	98
SELEXOL UNIT	Kwe	19,957	-
DESULFURIZER UNIT	Kwe	-	2,068
GAS TURBINE AUXILIARIES	Kwe	929	929
STEAM TURBINE AUXILIARIES	Kwe	114	111
CLAUS & TAIL GAS TREATING AUXILIARIES	Kwe	79	-
H2SO4 UNIT	Kwe	-	-1,535
MISCELLANEOUS BALANCE OF PLANT	Kwe	3,028	3,102
TRANSFORMER LOSSES	Kwe	2,567	2,538
NET PLANT EFFICIENCY, HHV	%	31.35	32.90
NET HEAT RATE	KJ/KWH	11,485	10,942
	BTU/KWH	10,885	10,371
CONDENSER COOLING DUTYNET	10^6 KJ/H	735	612
	10^6 BTU/H	696	580
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	295,046	302,251
	LB/H	650,575	666,462
THERMAL INPUT	KWT HHV	1,632,443	1,672,307
RAW WATER USAGE	M^3/MIN	14.42	15.96
	GPM	3,809	4,216
CARBON CAPTURED	%	90	90

Table 26. Overall Plant Performance Summary: Lignite Coal Cases Fully Loaded GTs.

CASE DESIGNATION	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	kWe	456,600	456,600
STEAM TURBINE POWER	kWe	289,856	299,807
TOTAL GROSS POWER	kWe	746,456	756,407
TOTAL AUXILIARY CONSUMPTION	kWe	241,194	158,416
NET POWER OUTPUT	kWe	505,262	597,992
AUXILIARY LOAD SUMMARY			
COAL HANDLING	kWe	848	934
COAL MILLING	kWe	4,300	4,731
COAL SLURRY PUMPS	kWe	859	946
SLAG HANDLING & DEWATERING	kWe	2,150	2,366
AIR SEPARATION UNIT AUXILIARIES	kWe	1,472	1,643
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	kWe	92,751	55,572
OXYGEN COMPRESSOR	kWe	15,084	35,424
NITROGEN COMPRESSOR	kWe	52,395	310
SYNGAS RECYCLE COMPRESSOR	kWe	559	614
TAIL GAS RECYCLE COMPRESSOR	kWe	1,808	-
CO ₂ PURIFICATION & COMPRESSION	kWe	22,670	30,410
BOILER FEEDWATER & DEMIN PUMPS	kWe	4,943	5,971
VACUUM CONDENSATE PUMP	kWe	304	334
PROCESS CONDENSATE & SWS SYSTEMS	kWe	366	1,018
HUMIDIFIER & BFW CIRCULATING PUMPS	kWe	28	152
COOLING WATER CIRCULATING PUMPS	kWe	4,175	3,579
COOLING TOWER + AIR COOLER FANS	kWe	5,758	4,923
SCRUBBER PUMPS	kWe	135	149
SELEXOL UNIT	kWe	22,328	-
DESULFURIZER UNIT	kWe	-	2,718
GAS TURBINE AUXILIARIES	kWe	984	984
STEAM TURBINE AUXILIARIES	kWe	126	130
CLAUS & TAIL GAS TREATING AUXILIARIES	kWe	96	-
H ₂ SO ₄ UNIT	kWe	-	-2,012
MISCELLANEOUS BALANCE OF PLANT	kWe	4,289	4,719
TRANSFORMER LOSSES	kWe	2,765	2,802
NET PLANT EFFICIENCY, HHV	%	28.28	30.42
NET HEAT RATE	KJ/KWH	12,731	11,836
	BTU/KWH	12,067	11,219
CONDENSER COOLING DUTY NET POWER	10 ⁶ KJ/H	816	696
	10 ⁶ BTU/H	773	660
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	417,873	459,799
	LB/H	921,411	1,013,856
THERMAL INPUT	KWT HHV	1,786,398	1,965,628
RAW WATER USAGE	M ³ /MIN	17.22	21.07
	GPM	4,550	5,567
CARBON CAPTURED	%	90	90

Table 27. Overall Plant Performance Summary: Subbituminous Coal Cases – Coal feed rate of 292,295 kg/h (as received).

	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	Kwe	426,882	416,707
STEAM TURBINE POWER	Kwe	259,612	245,935
TOTAL GROSS POWER	Kwe	686,494	662,642
TOTAL AUXILIARY CONSUMPTION	Kwe	179,424	130,420
NET POWER OUTPUT	Kwe	507,071	532,222
AUXILIARY LOAD SUMMARY			
COAL HANDLING	Kwe	593	593
COAL MILLING	Kwe	3,008	3,008
COAL SLURRY PUMPS	Kwe	652	652
SLAG HANDLING & DEWATERING	Kwe	1,485	1,484
AIR SEPARATION UNIT AUXILIARIES	Kwe	1,151	1,179
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	Kwe	65,121	47,785
OXYGEN COMPRESSOR	Kwe	15,433	22,901
NITROGEN COMPRESSOR	Kwe	29,662	7,721
SYNGAS RECYCLE COMPRESSOR	Kwe	515	515
TAIL GAS RECYCLE COMPRESSOR	Kwe	1,569	-
CO ₂ PURIFICATION & COMPRESSION	Kwe	20,155	24,659
BOILER FEEDWATER & DEMIN PUMPS	Kwe	4,417	4,730
VACUUM CONDENSATE PUMP	Kwe	280	280
PROCESS CONDENSATE & SWS SYSTEMS	Kwe	233	561
BFW CIRCULATING PUMPS	Kwe	23	94
COOLING WATER CIRCULATING PUMPS	Kwe	3,379	2,867
COOLING TOWER + AIR COOLER FANS	Kwe	5,227	4,322
SCRUBBER PUMPS	Kwe	94	94
SELEXOL UNIT	Kwe	19,771	-
DESULFURIZER UNIT	Kwe	-	1,999
GAS TURBINE AUXILIARIES	Kwe	920	898
STEAM TURBINE AUXILIARIES	Kwe	113	107
CLAUS & TAIL GAS TREATING AUXILIARIES	Kwe	78	-
H ₂ SO ₄ UNIT	Kwe	-	-1,485
MISCELLANEOUS BALANCE OF PLANT	Kwe	3,000	3,000
TRANSFORMER LOSSES	Kwe	2,543	2,454
NET PLANT EFFICIENCY, HHV	%	31.35	32.90
NET HEAT RATE	KJ/KWH	11,485	10,942
	BTU/KWH	10,885	10,371
CONDENSER COOLING DUTYNET POWER	10 ⁶ KJ/H	728	592
	10 ⁶ BTU/H	690	561
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	292,295	292,295
	LB/H	644,510	644,510
THERMAL INPUT	KWT HHV	1,617,223	1,617,224
RAW WATER USAGE	M ³ /MIN	14.28	15.43
	GPM	3,774	4,077
CARBON CAPTURED	%	90	90

Table 28. Overall Plant Performance Summary: Lignite Coal Cases – Coal feed rate of 292,295 kg/h (as received).

CASE DESIGNATION	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	kWe	319,383	290,262
STEAM TURBINE POWER	kWe	202,749	190,588
TOTAL GROSS POWER	kWe	522,132	480,850
TOTAL AUXILIARY CONSUMPTION	kWe	168,711	100,705
NET POWER OUTPUT	kWe	353,421	380,145
AUXILIARY LOAD SUMMARY			
COAL HANDLING	kWe	593	593
COAL MILLING	kWe	3,008	3,008
COAL SLURRY PUMPS	kWe	601	601
SLAG HANDLING & DEWATERING	kWe	1,504	1,504
AIR SEPARATION UNIT AUXILIARIES	kWe	1,030	1,044
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	kWe	64,878	35,327
OXYGEN COMPRESSOR	kWe	10,551	22,519
NITROGEN COMPRESSOR	kWe	36,649	197
SYNGAS RECYCLE COMPRESSOR	kWe	391	390
TAIL GAS RECYCLE COMPRESSOR	kWe	1,264	-
CO2 PURIFICATION & COMPRESSION	kWe	15,857	19,332
BOILER FEEDWATER & DEMIN PUMPS	kWe	3,457	3,795
VACUUM CONDENSATE PUMP	kWe	213	213
PROCESS CONDENSATE & SWS SYSTEMS	kWe	256	647
HUMIDIFIER & BFW CIRCULATING PUMPS	kWe	20	96
COOLING WATER CIRCULATING PUMPS	kWe	2,920	2,275
COOLING TOWER + AIR COOLER FANS	kWe	4,027	3,129
SCRUBBER PUMPS	kWe	94	94
SELEXOL UNIT	kWe	15,618	-
DESULFURIZER UNIT	kWe	-	1,728
GAS TURBINE AUXILIARIES	kWe	688	626
STEAM TURBINE AUXILIARIES	kWe	88	83
CLAUS & TAIL GAS TREATING AUXILIARIES	kWe	67	-
H2SO4 UNIT	kWe	-	-1,279
MISCELLANEOUS BALANCE OF PLANT	kWe	3,000	3,000
TRANSFORMER LOSSES	kWe	1,934	1,781
NET PLANT EFFICIENCY, HHV	%	28.28	30.42
NET HEAT RATE	KJ/KWH	12731.317	11836.35
	BTU/KWH	12066.96	11218.695
CONDENSER COOLING DUTY NET POWER	10^6 KJ/H	570.703	442.657
	10^6 BTU/H	540.922	419.557
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	292294.648	292294.97
	LB/H	644509.699	644510.408
THERMAL INPUT	KWT HHV	1249551.914	1249553.288
RAW WATER USAGE	M^3/MIN	12.046	13.395
	GPM	3182.659	3539.019
CARBON CAPTURED	%	89.927	90.002

Table 29. Overall Plant Cost Summary: Subbituminous Coal Cases – Fully Loaded GTs.

	COLD GAS CLEANUP	WARM GAS CLEANUP
UNIT	2007 Installed Cost (\$1000)	2007 Installed Cost (\$1000)
ASU	227,712	235,526
Fuel receiving, preparation & feeding	112,478	114,393
Gasifier, syngas cooler & aux	311,596	316,903
Other Gasification Equipments	68,092	69,252
Syngas scrubber (included in gasification auxiliaries)	0	0
Ash handling systems	39,849	40,528
Shift reactor	15,603	-
Hg Removal	3,147	-
Acid gas removal	207,362	-
Elemental Sulfur Plant	17,939	-
CO2 compression, dehydration & pumping	29,069	-
1st Shift reactor + Combined 2nd Shift & PSA + CO2 compression, dehydration & pumping	-	202,493
Warm gas desulfurization	-	13,440
H2SO4 unit	-	29,363
Blowback gas systems	3,281	3,337
Fuel gas piping	1,690	2,475
Gas cleanup foundations	1,789	3,573
Syngas Humidification	0	-
N2 Humidification	-	2,727
Gas turbine + generator + auxiliaries	132,424	132,424
HRSG, ducting + stack	54,871	55,233
Steam turbine + generator + auxiliaries	54,238	53,111
Surface condenser	30,008	26,415
Feedwater & Misc. BOP Systems	38,194	69,868
Cooling water system	26,858	26,986
Accessory electric plant	90,559	89,849
Instrumentation & controls	27,364	27,364
Improvement to site	19,590	19,924
Buildings & structures	18,471	18,785
Total	1,532,182	1,553,969
Total \$/kW	2,993	2,824

Table 30. Overall Plant Cost Summary: Lignite Coal Cases – Fully Loaded GTs.

	COLD GAS CLEANUP	WARM GAS CLEANUP
UNIT	2007 Installed Cost (\$1000)	2007 Installed Cost (\$1000)
ASU	278,625	290,122
Fuel receiving, preparation & feeding	143,508	153,441
Gasifier, syngas cooler & aux	331,887	354,859
Other Gasification Equipments	72,526	77,546
Syngas scrubber (included in gasification auxiliaries)	0	0
Ash handling systems	57,895	61,903
Shift reactor	17,697	-
Hg Removal	3,252	-
Acid gas removal	224,323	-
Elemental Sulfur Plant	20,613	-
CO2 compression, dehydration & pumping	31,356	-
1st Shift reactor + Combined 2nd Shift & PSA + CO2 compression, dehydration & pumping	-	229,531
Warm gas desulfurization	-	16,229
H2SO4 unit	-	35,459
Blowback gas systems	3,495	3,737
Fuel gas piping	1,685	3,044
Gas cleanup foundations	2,029	4,313
Gas turbine + generator + auxiliaries	137,904	137,904
HRSG, ducting + stack	53,463	57,283
Steam turbine + generator + auxiliaries	58,204	59,596
Surface condenser	32,293	28,902
Feedwater & Misc. BOP Systems	31,893	79,629
Cooling water system	25,585	27,777
Accessory electric plant	95,398	96,287
Instrumentation & controls	27,364	27,364
Improvement to site	20,866	22,310
Buildings & structures	19,674	21,035
Total	1,691,535	1,788,271
Total \$/kW	3,348	2,990

Table 31. Cost of Electricity: Subbituminous Coal Cases – Fully Loaded GTs 2007 \$.

	COLD GAS CLEANUP	WARM GAS CLEANUP
Net power, MW	511.84	550.35
Capacity factor (CF), %	80	80
Total plant cost (TPC), \$	1,532,182,156	1,553,969,441
6 month labor cost	14,259,309	14,449,993
1 month maintenance materials	2,553,786	2,601,003
1 month non-fuel consumables	376,323	787,430
1 month waste disposal	335,045	415,373
25% of 1 month fuel cost at 100% CF	903,691	925,758
2% of TPC	30,643,643	31,079,389
60 day supply of fuel & consumables at 100% CF	7,872,830	8,857,898
0.5% of TPC (spare parts)	7,660,911	7,769,847
Initial catalyst & chemicals cost, \$	7,295,886	13,388,363
Land	900,000	900,000
Other owners's costs	229,827,323	233,095,416
Financing costs	41,368,918	41,957,175
Total overnight cost (TOC), \$	1,876,179,821	1,910,197,085
Fixed operating cost for initial year of operation (OCF), \$	59,162,262	59,979,374
Annual feed cost at above CF for initial year (OCV1), \$	34,701,738	35,549,111
Other annual variable operating cost at above CF for initial year (OCV2), \$	31,345,478	36,516,530
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year (OCV3), \$	20,696,359	21,171,852
Annual byproduct revenues at above CF for initial year (OCV4), \$	1,491,218	4,666,995
1st year cost of electricity (COE) w/o CO2 TS&M, \$/MWh	99.5	94.6
1st year cost of electricity (COE), \$/MWh	105.3	100.1

Table 32. Cost of Electricity: Lignite Coal Cases – Fully Loaded GTs 2007 \$.

	COLD GAS CLEANUP	WARM GAS CLEANUP
Net power, MW	505.26	597.99
Capacity factor (CF), %	80	80
Total plant cost (TPC), \$	1,691,535,249	1,788,271,144
6 month labor cost	15,279,234	16,010,475
1 month maintenance materials	2,806,339	2,987,408
1 month non-fuel consumables	360,219	914,213
1 month waste disposal	568,434	718,628
25% of 1 month fuel cost at 100% CF	918,298	1,010,430
2% of TPC	33,830,705	35,765,423
60 day supply of fuel & consumables at 100% CF	7,956,319	9,776,087
0.5% of TPC (spare parts)	8,457,676	8,941,356
Initial catalyst & chemicals cost, \$	8,387,100	16,606,225
Land	900,000	900,000
Other owners's costs	253,730,287	268,240,672
Financing costs	45,671,452	48,283,321
Total overnight cost (TOC), \$	2,070,401,313	2,198,425,380
Fixed operating cost for initial year of operation (OCF), \$	64,389,173	67,786,373
Annual feed cost at above CF for initial year (OCV1), \$	35,262,646	38,800,513
Other annual variable operating cost at above CF for initial year (OCV2), \$	35,855,926	44,354,385
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year (OCV3), \$	23,134,685	25,324,381
Annual byproduct revenues at above CF for initial year (OCV4), \$	1,818,599	6,127,517
1st year cost of electricity (COE) w/o CO2 TS&M, \$/MWh	110.4	99.8
1st year cost of electricity (COE), \$/MWh	117.0	105.8

3.7.1 Subbituminous Coal Cases

The calculated net thermal efficiency of the Warm Gas Cleanup Case is significantly higher at 32.90% versus 31.35% (on a coal HHV basis) for the Cold Gas Cleanup Case.

On a constant coal throughput basis, the cold gas capture case produced higher total power than warm gas capture. This is due to more power being generated in the gas turbine for the cold gas cleanup case. Water vapor is the major diluent present in the syngas entering gas turbine in the warm gas cleanup case while N₂ from ASU is the major diluent present in the syngas entering the gas turbine in the cold gas cleanup case. Less amount of water vapor is required to achieve the same level of NO_x emissions as with N₂. This reduces the gas turbine output for the warm gas cleanup case when expressed on a unit coal flow basis.

However, the net power produced is higher for the warm gas cleanup with lower auxiliary loads (134,862 kWe) in the case of warm gas cleanup with TDA's combined shift and CO₂ capture system compared to cold gas cleanup (181,112 kWe) with Selexol™ providing a net difference in auxiliary load of 46.25 MWe. There are two major subsystems that result in this reduction in auxiliary load for the warm gas cleanup case: the ASU and the CO₂ capture and sulfur removal system.

In the case of the ASU the power consumption (air, O₂ and N₂ compression + auxiliaries) for cold gas cleanup case is very high (112.41 MWe) compared to warm gas cleanup case (82.30 MWe) (a net difference of 30.11 MWe). The ASU was modeled as comprising a low pressure (LP) ASU and an elevated pressure (EP) ASU for both the cases. The relative size of these two units is set by the amount of nitrogen required for gas turbine injection to minimize compression of air. The warm gas cleanup case requires less nitrogen for gas turbine and thus the size of the EP ASU unit is smaller (while that of the LP ASU is larger) when compared to cold gas cleanup case. Hence the auxiliary load for air compression is higher for cold gas cleanup case. Also the diluent N₂ supplied by the ASU to the gas turbine requires a significant amount of compression (from the pressure leaving the elevated pressure cold box to that required by the gas turbine). Hence the auxiliary load for the nitrogen compressor is higher for cold gas capture. However, the auxiliary load for oxygen compressor is higher for warm gas cleanup case since more oxygen from the LP ASU needs to be compressed for use in the gasifier and the catalytic combustor.

The auxiliary load for CO₂ separation, purification and compression and sulfur removal for the warm gas cleanup case with TDA's combined shift and high temperature PSA system is significantly lower at 26.03 MWe compared to 40.38 MWe for cold gas cleanup with Selexol™ (a net difference of 14.35 MWe). The above results indicate that warm gas cleanup technology coupled with the combined shift and CO₂ adsorption process being developed by TDA can make a substantial improvement in the IGCC plant thermal performance designed for approaching near zero emissions, i.e., to include CO₂ capture.

The plant cost for the Warm gas Cleanup Case is \$2824/kW while that for the Cold Gas Case is \$2993/kW, or a decrease of about 6% over the Cold Gas Cleanup Case. The levelized cost of electricity with transport, storage and monitoring (TS&M) costs for the CO₂ included is \$100.1/MWh for the Warm gas Cleanup Case while that for the Cold Gas Case is \$105.3/MWh, or a decrease of about 5% over the Cold Gas Cleanup Case.

3.7.2 Lignite Coal Cases

The calculated net thermal efficiency of the Warm Gas Cleanup Case is significantly higher at 30.42% versus 28.28% (on a coal HHV basis) for the Cold Gas Cleanup Case.

On a constant coal throughput basis, the cold gas capture case produced higher total power than warm gas capture. This is due to more power being generated in the gas turbine for the cold gas cleanup case. Water vapor is the major diluent present in the syngas entering gas turbine in the warm gas cleanup case while N₂ from ASU is the major diluent present in the syngas entering the gas turbine in the cold gas cleanup case. Less amount of water vapor is required to achieve the same level of NO_x emissions as with N₂. This reduces the gas turbine output for the warm gas cleanup case when expressed on a unit coal flow basis.

However, the net power produced is higher for the warm gas cleanup with lower auxiliary loads (158,416 kWe) in the case of warm gas cleanup with TDA's combined shift and CO₂ capture system compared to cold gas cleanup (241,194 kWe) with Selexol™ providing a net difference in auxiliary load of 82.78 MWe. There are two major subsystems that result in this reduction in auxiliary load for the warm gas cleanup case: the ASU and the CO₂ capture and sulfur removal system.

In the case of the ASU the power consumption for cold gas cleanup case is very high (161.70 MWe) compared to warm gas cleanup case (84.47 MWe) (a net difference of 77.23 MWe). The ASU was modeled as comprising a low pressure (LP) ASU and an elevated pressure (EP) ASU for both the cases. The relative size of these two units is set by the amount of nitrogen required for gas turbine injection to minimize compression of air. The warm gas cleanup case requires less nitrogen for gas turbine and thus the size of the EP ASU unit is smaller (while that of the LP ASU is larger) when compared to cold gas cleanup case. Hence the auxiliary load for air compression is higher for cold gas cleanup case. Also the diluent N₂ supplied by the ASU to the gas turbine requires a significant amount of compression (from the pressure leaving the elevated pressure cold box to that required by the gas turbine). Hence the auxiliary load for the nitrogen compressor is higher for cold gas capture. However, the auxiliary load for oxygen compressor is higher for warm gas cleanup case since more oxygen from the LP ASU needs to be compressed for use in the gasifier and the catalytic combustor.

The auxiliary load for CO₂ separation, purification and compression and sulfur removal for the warm gas cleanup case with TDA's combined shift and high temperature PSA system is significantly lower at 28.28 MWe compared to 45.09 MWe for cold gas cleanup with Selexol™ (a net difference of 16.81 MWe).

The above results indicate that warm gas cleanup technology coupled with the combined shift and CO₂ adsorption process being developed by TDA can make a substantial improvement in the IGCC plant thermal performance designed for approaching near zero emissions, i.e., to include CO₂ capture.

The plant cost for the Warm gas Cleanup Case is \$2990/kW while that for the Cold Gas Case is \$3348/kW, or a decrease of as much as 11% over the Cold Gas Cleanup Case. The levelized cost of electricity with transport, storage and monitoring (TS&M) costs for the CO₂ included is \$105.8/MWh for the Warm gas Cleanup Case while that for the Cold Gas Case is \$117.0/MWh, or a decrease of about 10% over the Cold Gas Cleanup Case.

3.7.3 Summary of Process Design and System Analysis

The Warm Gas Cleanup system using TDA's combined shift and high temperature PSA-based CO₂ capture system achieved net plant efficiencies of 32.90% and 30.42% (on a coal HHV basis) for the subbituminous and the lignite coals. These net plant efficiencies at 90% carbon capture are significantly higher than those achieved for the corresponding Cold Gas Cases using Selexol™ scrubber at 31.35% and 28.28% (on a coal HHV basis for the subbituminous and the lignite coals respectively) which correspond to about 5% and 7% decrease in the heat rate respectively for TDA's Warm Gas Cleanup system.

The capital expense for the plants were estimated following the "Cost Guidelines provide by DOE/NETL (2007) (e.g. higher contingencies were applied for unproven technologies such as the combined shift and high temperature PSA unit). The plant cost for TDA's Warm gas Cleanup Process is estimated as \$2824/kW and \$2990/kW for the subbituminous and the lignite coals, which are about 6% and 11% lower than those of the corresponding Cold Gas Cleanup Cases at \$2993/kW and \$3348/kW (for the subbituminous and the lignite coals respectively). The levelized cost of electricity including the transport, storage and monitoring (TS&M) costs for CO₂ is calculated as \$100.1/MWh and \$105.8/MWh for the subbituminous and the lignite coal cases with TDA's Warm gas Cleanup technology. The corresponding costs for the Cold Gas Cases using the Selexol™ scrubbing technology are calculated as \$105.3/MWh and \$117.0/MWh (for the subbituminous and the lignite coals respectively).

Table 33. Comparison of TDA's Warm Gas Cleanup against Selexol™ based Cold Gas Cleanup System with fully loaded GE F class type gas turbines.

Coal Type	Subbituminous		Lignite	
	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent
Raw Gas Cleanup Option				
CO ₂ Capture, %	90	90	90	90
Gross Power Generated, kWe	692,955	685,211	746,456	756,407
Gas Turbine Power	430,900	430,900	456,600	456,600
Steam Turbine Power	262,055	254,311	289,856	299,807
Auxiliary Load, kWe	181,112	134,862	241,194	158,416
Net Power, kWe	511,843	550,349	505,262	597,992
Net Plant Efficiency, % HHV	31.35	32.90	28.28	30.42
Coal Feed Rate, kg/h	295,046	302,251	417,873	459,799
Raw Water Usage, GPM/MWe	7.4	7.7	9.0	9.3
Total Plant Cost, \$/kWe	2,993	2,824	3,348	2,990
COE without CO ₂ TS&M, \$/MWh	99.5	94.6	110.4	99.8
COE with CO ₂ TS&M, \$/MWh	105.3	100.1	117.0	105.8

The results of the system analysis suggest that TDA's combined shift and high temperature PSA-based Warm Gas Clean-up technology can make a substantial improvement in the IGCC plant thermal performance for achieving near zero emissions (including greater than 90% carbon capture). The capital expenses are also expected to be lower than those of Selexol's™. The higher net plant efficiency and lower capital and operating costs result in substantial

reduction in the COE for the IGCC plant equipped with TDA's combined shift and high temperature PSA-based carbon capture system.

4. Conclusions and Recommendations

In this project we developed a new pre-combustion carbon capture technology that combines the 2nd & 3rd stage water gas shift reaction with a CO₂ capture technology that operates above the dewpoint of the synthesis gas and demonstrated its technical feasibility and economic viability in laboratory-scale tests and field demonstrations and carried out a detailed process design and analysis of the new system as part of an Integrated Gasification Combined Cycle (IGCC) power plant operating on low rank coals such as Sub-bituminous and lignite. The new technology uses a low cost, high capacity adsorbent that selectively removes CO₂ above the dew point of the synthesis gas (190 to 260°C is explored in this study depending on the gasifier type). The sorbent is based on a TDA proprietary mesoporous carbon that consists of surface functionalized groups that remove CO₂ via physical adsorption. The high surface area and favorable porosity of the sorbent also provide a unique platform to introduce additional functionality, such as active groups to remove trace metals (e.g., Hg, As) in the same bed and also the operating temperatures allows us to carry out sorbent enhanced water gas shift reaction.

In collaboration with the Advanced Power and Energy Program of the University of California, Irvine (UCI), TDA developed system simulation models using Aspen PlusTM simulation software to assess the economic viability of TDA's high temperature PSA-based pre-combustion carbon capture technology. The simulation results showed that the CO₂ product purity from TDA's combined WGS and high temperature PSA system at 90% carbon capture could match the purity levels that can be achieved by the SelexolTM process. TDA's combined shift and high temperature PSA-based CO₂ capture system achieved net plant efficiencies of 32.90% and 30.42% (on a coal HHV basis) for the subbituminous and the lignite coals. These net plant efficiencies at 90% carbon capture are significantly higher than those achieved for the corresponding Cold Gas Cases using SelexolTM scrubber at 31.35% and 28.28% (on a coal HHV basis for the subbituminous and the lignite coals respectively) which correspond to about 5% and 7% decrease in the heat rate respectively for TDA's Warm Gas Cleanup system. The plant cost for TDA's Warm gas Cleanup Process is estimated as \$2824/kW and \$2990/kW for the subbituminous and the lignite coals, which are about 6% and 11% lower than those of the corresponding Cold Gas Cleanup Cases at \$2993/kW and \$3348/kW (for the subbituminous and the lignite coals respectively). The levelized cost of electricity including the transport, storage and monitoring (TS&M) costs for CO₂ is calculated as \$100.1/MWh and \$105.8/MWh for the subbituminous and the lignite coal cases with TDA's Warm gas Cleanup technology. The corresponding costs for the Cold Gas Cases using the SelexolTM scrubbing technology are calculated as \$105.3/MWh and \$117.0/MWh (for the subbituminous and the lignite coals respectively).

The results of the system analysis suggest that TDA's high temperature PSA-based Warm Gas Clean-up Technology can make a substantial improvement in the IGCC plant thermal performance for units that are designed to produce near zero emissions, including greater than 90% carbon capture. The capital expenses are also expected to be lower than that of Selexol'sTM. The higher net plant efficiency and lower capital and operating costs results in substantial reduction in the cost of electricity for the IGCC plant equipped with TDA's high temperature PSA-based carbon capture system.

4.1 Recommendations for Future Work

The results of the DE-FE0007966 project suggest that the combined WGS and high temperature PSA-based pre-combustion carbon capture technology has merits for further research and development. It is recommended that detailed CFD modeling of the combined WGS and high temperature PSA reactors to optimize the ratio of Shift reaction that takes place in the CO₂ sorbent beds and also to have an advanced reactor design to provide optimal heat management when the two exothermic processes i.e., WGS reaction and CO₂ removal by adsorption are combined in the single bed. The performance of the advanced reactor design needs to be validated using actual coal derived synthesis gas and also a fully-equipped system should be demonstrated at larger-scale (e.g., 0.1 to 1 MW) using actual synthesis gas for a longer duration (6 to 12 months). The system should contain all critical components (including all PSA reactors, accumulators etc.) to fully demonstrate the cycle sequence, enabling the demonstration of product purity (both the hydrogen-rich fuel gas and CO₂-rich retentate). The demonstration duration should be long enough to allow over 20,000 cycles (with a 16 min full cycle time it corresponds to 7.5 months of testing) under optimum operating conditions. The selected demonstration scale should be large enough require sorbent production in large quantities (at the recommended 1 MW demonstration 8 m³ of sorbent will be needed). A more detailed system simulation and cost analysis is also recommended, including design work and accurate quotes from the suppliers of the major process equipment (e.g., air separation unit, gasifier, CO₂ compressors). Successful completion of this recommended work will provide the basis for the new technology to be employed in potential commercial pilot-scale demonstrations (50-100 MW scale).

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Nomenclature

B	langmuir parameter, atm^{-1}
D_{ax}	axial dispersion coefficient, m^2/s
D_e/r^2	diffusional time constant, s^{-1}
$-\Delta H$	Heat of adsorption, kcal/mol
L	length of the adsorption column, m
n	Langmuir-Freundlich constant
P	pressure, atm or bar
P_{CBD}	pressure at the end of countercurrent blowdown step, bar
P_{CO_2}	partial pressure of CO_2 , atm or bar
P_{DES}	pressure at the end of desorption step, bar
P_H	pressure in the adsorption step, bar
q	adsorbed phase concentration, mmol/g or $\% \text{ wt. CO}_2$
q_s	adsorbed phase concentration at saturation, mmol/g or $\% \text{ wt. CO}_2$
$\bar{q}$	equilibrium adsorbed phase concentration, mmol/g
q	average adsorbed phase concentration, mmol/g
q_m	maximum adsorbed phase concentration, mmol/g
R	radius of the spherical particle, m
t	time, s
T	temperature, K
u	gas phase velocity, m/s
z	axial position in the bed, m
ε	bed porosity due to packing
ε_t	total bed porosity including macropores

Appendix A

Aspen Model and Simulation Results for Advanced CO₂ Capture
Technology for Low rank Coal IGCC prepared by UCI

**TDA
DOE Contract DE-FOA0007966**

FINAL REPORT

Advanced CO₂ Capture Technology for Low rank Coal IGCC

Prepared By

Advanced Power and Energy Program

**University of California, Irvine
*September 2013***

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1.0 Executive Summary

Since half of the coal in the United States is low rank coal, and its use is expected to grow significantly, a worthwhile development path is to evolve advanced technology for the use of low rank coal in power production. The overall objective for this project is the development of low rank coal gasification technologies resulting in economically viable production of power with a potential to cause a significant reduction in the cost of electricity (COE) with carbon capture and sequestration (CCS) as compared to the state-of-the-art and commercially available Integrated Gasification Combined Cycle (IGCC) technologies. The gasifier selected for use in the proposed design concept is the commercially available Phillips 66 gasifier. Concepts with the widest applicability to the IGCC industry will be favored over those with a narrow scope.

The advanced technology combines simultaneous shifting of the syngas with a low cost, high capacity adsorbent that selectively removes CO₂ above the dew point of the synthesis gas. The sorbent regeneration is carried out using a combination of pressure swing (i.e., reducing the pressure to 10 barA) and concentration swing by using steam purge per regeneration while maintaining near isothermal operation. The near isothermal conditions are maintained by equipping the vessels with internal heat transfer tubes that generate steam. The high temperature pressure swing adsorption (PSA) unit also removes trace metal contaminants (such as Hg and As) and when combined with warm gas desulfurization cleanup provides a complete warm gas clean-up platform for IGCC plants. For a nominal 600 MW IGCC plant, the CO₂ removal system consists of three trains of 8-bed shift/PSA units (total of 24 beds housing the shift catalyst and the CO₂ sorbent) that undergo a PSA sequence, including adsorption, depressurization, pressure equalization, desorption and steam purge; all of which ensure continuous removal of CO₂ from the synthesis gas, generating a concentrated CO₂ stream ready for further purification and compression and also a very low CO₂ containing synthesis gas fuel to be combusted in the gas turbine.

Under subcontract to TDA Research, the Advanced Power and Energy Program of the University of California, Irvine (UCI), provided assistance in the process design and developed system simulation models to assess the economic viability of TDA's combined shift and high temperature PSA-based pre-combustion carbon capture (Warm Gas Cleanup) technology. The analysis also provided thorough comparison against the conventional cold gas cleanup technology utilizing the Selexol™ physical solvent scrubbing (used for desulfurization and decarbonization of the raw syngas). The gasification system performance was provided by Phillips 66 for the two low rank coals studied: Powder River Basin (PRB) subbituminous coal from Montana and lignite coal from North Dakota. These data consisted of the definition of all key process parameters including the gas composition, flow rate, temperature and pressure of each process stream entering and leaving each of the gasification systems (from the incoming coal slurry and oxygen to the outgoing raw scrubbed syngas). The performance data for the combined shift and CO₂ removal system was provided by TDA that consisted again of the definition of all key process parameters including the gas composition, flow rate, temperature and pressure of each process stream entering and leaving this combined system. UCI then developed the overall process model with all sub-systems for the two site specific conditions. Prior to the process design and modeling, the accuracy of the Aspen Plus® model was verified by checking simulation results against the data provided by Phillips 66.

The Warm Gas Cleanup system using TDA's combined shift and high temperature PSA-based CO₂ capture system achieved net plant efficiencies of 32.90% and 30.42% (on a coal HHV basis) for the subbituminous and the lignite coals. These net plant efficiencies at 90% carbon capture are significantly higher than those achieved for the corresponding Cold Gas Cases using Selexol™ scrubber at 31.35% and 28.28% (on a coal HHV basis for the subbituminous and the lignite coals respectively) which correspond to about 5% and 7% decrease in the heat rate respectively for TDA's Warm Gas Cleanup system.

The capital expense for the plants were estimated following the "Cost Guidelines provide by DOE/NETL (2007) (e.g. higher contingencies were applied for unproven technologies such as the combined shift and high temperature PSA unit). The plant cost for TDA's Warm gas Cleanup Process is estimated as \$2824/kW and \$2990/kW for the subbituminous and the lignite coals, which are about 6% and 11% lower than those of the corresponding Cold Gas Cleanup Cases at \$2993/kW and \$3348/kW (for the subbituminous and the lignite coals respectively). The levelized cost of electricity including the transport, storage and monitoring (TS&M) costs for CO₂ is calculated as \$100.1/MWh and \$105.8/MWh for the subbituminous and the lignite coal cases with TDA's Warm gas Cleanup technology. The corresponding costs for the Cold Gas Cases using the Selexol™ scrubbing technology are calculated as \$105.3/MWh and \$117.0/MWh (for the subbituminous and the lignite coals respectively).

Table 1-1: Comparison of TDA's Warm Gas Cleanup against Selexol™ based Cold Gas Cleanup System with fully loaded GE F class type gas turbines

Coal Type	Subbituminous		Lignite	
	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent	Cold Gas Cleanup Selexol™	Warm Gas Cleanup TDA's CO ₂ Sorbent
Raw Gas Cleanup Option				
CO ₂ Capture, %	90	90	90	90
Gross Power Generated, kWe	692,955	685,211	746,456	756,407
Gas Turbine Power	430,900	430,900	456,600	456,600
Steam Turbine Power	262,055	254,311	289,856	299,807
Auxiliary Load, kWe	181,112	134,862	241,194	158,416
Net Power, kWe	511,843	550,349	505,262	597,992
Net Plant Efficiency, % HHV	31.35	32.90	28.28	30.42
Coal Feed Rate, kg/h	295,046	302,251	417,873	459,799
Raw Water Usage, GPM/MWe	7.4	7.7	9.0	9.3
Total Plant Cost, \$/kWe	2,993	2,824	3,348	2,990
COE without CO ₂ TS&M, \$/MWh	99.5	94.6	110.4	99.8
COE with CO ₂ TS&M, \$MWH	105.3	100.1	117.0	105.8

The results of the system analysis suggest that TDA's combined shift and high temperature PSA-based Warm Gas Clean-up technology can make a substantial improvement in the IGCC plant thermal performance for achieving near zero emissions (including greater than 90% carbon capture). The capital expenses are also expected to be lower than those of Selexol's™. The higher net plant efficiency and lower capital and operating costs result in substantial

reduction in the COE for the IGCC plant equipped with TDA's combined shift and high temperature PSA-based carbon capture system.

2.0 Introduction

The overall objective of this project is to develop a new pre-combustion carbon capture technology and demonstrate its technical feasibility and economic viability and carrying out detailed process design and analysis as part of an IGCC power plant. The advanced technology combines simultaneous shifting of the syngas with a low cost, high capacity adsorbent that selectively removes CO₂ above the dew point of the synthesis gas. The sorbent regeneration is carried out using a combination of pressure swing (i.e., reducing the pressure to 10 barA) and concentration swing by using steam purge per regeneration while maintaining near isothermal operation. The near isothermal conditions are maintained by equipping the vessels with internal heat transfer tubes that generate steam. The high temperature pressure swing adsorption (PSA) unit also removes trace metal contaminants (such as Hg and As) and when combined with warm gas desulfurization cleanup provides a complete warm gas clean-up platform for IGCC plants. For a nominal 600 MW IGCC plant, the CO₂ removal system consists of three trains of 8-bed shift/PSA units (total of 24 beds housing the shift catalyst and the CO₂ sorbent) that undergo a PSA sequence, including adsorption, depressurization, pressure equalization, desorption and steam purge; all of which ensure continuous removal of CO₂ from the synthesis gas, generating a concentrated CO₂ stream ready for further purification and compression and also a very low CO₂ containing synthesis gas fuel to be combusted in the gas turbine.

2.1 IGCC Plant Integrated with TDA's Combined Shift and Regenerable Sorbent CO₂ Capture Process

Figure 2-1 shows a simplified block diagram of an IGCC plant integrated with TDA's combined shift and high temperature PSA-based CO₂ capture / purification process (blocks in green). TDA's Warm Gas CO₂ capture system is located downstream of a warm gas desulfurization system (we used the regenerable zinc-titanate-based syngas desulfurization system developed by the Research Triangle Institute). The regeneration off-gas from the desulfurization system is further treated in a sulfuric acid plant, ultimately converting all sulfur into a concentrated H₂SO₄ byproduct. The desulfurized synthesis gas is then fed to a first adiabatic shift reactor for the (partial) conversion of the CO into H₂. The synthesis gas from the first shift unit after heat recovery is then sent to the combined shift and CO₂ capture system at a temperature (at least 30°C) above the dew point of the syngas. The decarbonized syngas leaves this system with a significant amount of moisture in it and is fed to the gas turbines after preheating to maximize overall plant efficiency. The TDA's Warm Gas cleanup process thus eliminates the need to cool the synthesis gas below its dew point using condensing heat exchangers.

The CO₂ purification/compression system further treats the CO₂ stream from the separation unit into a high purity, pressurized CO₂ byproduct that meets pipeline specifications. Any gases trapped in the voids of the sorbent and the reactor ullage space are recovered at an intermediate pressure and recycled back to the syngas feed to ensure high H₂ recovery in the CO₂ separation unit. A steam purge at lower pressure is used to fully regenerate the sorbent. A CO₂ rich stream primarily consisting of H₂O and CO₂ (along with some CO and H₂ impurities) is sent for further purification consisting of a catalytic combustor to burn any residual syngas with

oxygen) and compression, liquefaction and pumping to produce a high purity CO₂ stream at 15.3 MPa (2,215 psia) that can be sent for sequestration.

Figure 2-1: TDA's CO₂ Separation System Integrated with an IGCC plant

2.2 TDA's CO₂ Separation System

Figure 2-2: Simplified block diagram of TDA's CO₂ removal unit

Simplified block diagram of TDA's warm gas CO₂ removal unit along with the various streams entering and leaving the system are shown in Figure 2-2. TDA provided the composition, pressure and temperature of these streams along with the bed sizing factor for sizing the sorbent requirement and the 3-D layout for the system. TDA's warm gas CO₂ capture system consists of three trains of 8-bed PSA systems containing a total of 24 beds that go through the following PSA cycle steps. A 3-D layout of the TDA's warm gas CO₂ capture system provided by TDA is shown in Figure 2-3.

Table 2-1: 8-bed PSA cycle steps 4 pressure equalizations and with co-depressurization

Step 1	Adsorption at 44.16 bar (ADS)
Step 2	Pressure Equalization to 36.4 bar (EQ1D)
Step 3	Pressure Equalization to 30.0 bar (EQ2D)
Step 4	Pressure Equalization to 23.2 bar (EQ3D)
Step 5	Pressure Equalization to 15.7 bar (EQ4D)
Step 6	Co-current Depressurization to 10.1 bar (CoDEP)
Step 7	Blowdown to 10 bar (BD)
Step 8	Steam Purge at 10 bar (PURGE)
Step 9	Pressure Equalization to 15.7 bar (EQ4R)
Step 10	Pressure Equalization to 23.2 bar (EQ3R)
Step 11	Pressure Equalization to 30.0 bar (EQ2R)
Step 12	Pressure Equalization to 36.4 bar (EQ1R)
Step 13	Product Pressurization to 44.16 bar (PRESS)

Figure 2-3: 3-D Layout of TDA's high temperature PSA-based CO₂ removal system showing the three trains of 8-PSA beds

3.0 Process Design Basis and Methodology

Consistency has been maintained between the IGCC case developed under this study utilizing the TDA's high temperature PSA-based CO₂ capture process (**Warm Gas Cleanup Cases**) with the Phillips 66 gasifier based IGCC plant with CO₂ capture utilizing current state-of-the-art syngas cleanup and CO₂ capture technology (**Cold Gas Cleanup Cases**).

The combined shifting and CO₂ adsorption in the Warm Gas Cleanup cases uses a shift catalyst along with TDA's low cost, high capacity CO₂ sorbent in the same vessel equipped with internal heat transfer tubes generating steam while maintaining near isothermal bed conditions. The sorbent can also simultaneously remove the trace contaminants such as Hg and As that are present in the synthesis gas. Performance data for the shifting and CO₂ adsorption unit (with co-sorption of Hg) were provided by TDA and consisted of the definition of the streams (composition, flow rate, temperature and pressure) associated with this subsystem for a partially shifted syngas stream (leaving the 1st shift reactor operated under adiabatic conditions) as estimated by UCI. Sizing basis for the combined shifting and CO₂ sorption vessels using the pressure swing adsorption (PSA) process was also provided by TDA.

3.1 Site Conditions

The plants are designed for the following mean ambient conditions which are the same as those in the previous DOE/NETL study (DOE/NETL-2010/1399):

Montana Site Ambient Conditions for PRB Coal Cases:

- Elevation, m (ft) = 1,036 (3,400)
- Barometric Pressure, MPa (psia) = 0.09 (13.0)
- Design Ambient Temperature, Dry Bulb, °C (°F) = 5.6 (42)
- Design Ambient Temperature, Wet Bulb, °C (°F) = 2.8 (37)
- Design Ambient Relative Humidity, % = 62

North Dakota Site Ambient Conditions for Lignite Coal Cases:

- Elevation, m (ft) = 579 (1,900)
- Barometric Pressure, MPa (psia) = 0.10 (13.8)
- Design Ambient Temperature, Dry Bulb, °C (°F) = 4.4 (40)
- Design Ambient Temperature, Wet Bulb, °C (°F) = 2.2 (36)
- Design Ambient Relative Humidity, % = 68

A parallel wet/dry condenser was chosen for all plant configurations since these plants are located in the Western U.S. and need to consider limited water supplies which is consistent with the previous DOE/NETL study (DOE/NETL-2010/1399). In this parallel cooling system, half of the turbine exhaust steam is condensed in an air-cooled condenser and the remaining half in a water-cooled condenser. The cooling water is provided by a mechanical draft, evaporative cooling tower.

The site characteristics are assumed to be the same for both plant locations which are the same as in the previous DOE/NETL study (DOE/NETL-2010/1399):

- Location: Greenfield
- Topography: Level
- Size, acres: 300
- Transportation: Rail
- Ash/Slag Disposal: Off Site
- Makeup Water: Municipal (50%) / Groundwater (50%)
- Access: Landlocked, having access by rail and highway
- CO₂ Storage: Compressed to 15.3 MPa (2,215 psia), transported 80 kilometers (50 miles) and sequestered in a saline formation at a depth of 1,239 meters (4,055 feet)

It is assumed that the land area required for all cases is 30 acres for the plant proper, and the balance provides a buffer of approximately 0.25 miles to the fence line. The extra land could also provide for a rail loop if required. In all cases it is assumed that the steam turbine is enclosed in a turbine building, but the gasifiers are not enclosed. The following design parameters are not quantified for this study as these are considered site-specific, and allowances only for normal conditions and construction are included in the cost estimates.

- Flood plain considerations
- Existing soil/site conditions
- Water discharges and reuse
- Rainfall/snowfall criteria
- Seismic design
- Buildings/enclosures
- Fire protection
- Local code height requirements
- Noise regulations – Impact on site and surrounding area

3.2 Coal Feed

The characteristics of the coal feed are the same as that in the previous DOE/NETL study (DOE/NETL-2010/1399) and are shown in Tables 3-1 and 3-2.

Table 3-1: Montana Rosebud PRB, Area D, Western Energy Co. Mine,
Subbituminous Design Coal Analysis

	Subbituminous	
Proximate Analysis	Dry Basis, %	As Received, %
Moisture	0	25.77
Ash	11.04	8.19
Volatile Matter	40.87	30.34
Fixed Carbon	48.09	35.7
Total	100	100
Ultimate Analysis	Dry Basis, %	As Received, %
Carbon	67.45	50.07
Hydrogen	4.56	3.38
Nitrogen	0.96	0.71
Sulfur	0.98	0.73
Chlorine	0.01	0.01
Ash	11.03	8.19
Moisture	0	25.77
Oxygen	15.01	11.14
Total	100	100
Heating Value	Dry Basis	As Received
HHV, kJ/kg	26,787	19,920
HHV, Btu/lb	11,516	8,564
LHV, kJ/kg	25,810	19,195
LHV, Btu/lb	11,096	8,252
Trace Components		
Mercury ¹ , ppm		0.081

¹ Mercury content is the mean plus one standard deviation using EPA's ICR data.

Table 3-2: North Dakota Beulah-Zap Lignite, Freedom, ND Mine,
Lignite Design Coal Analysis

	Lignite	
Proximate Analysis	Dry Basis, %	As Received, %
Moisture	0	36.08
Ash	15.43	9.86
Volatile Matter	41.49	26.52
Fixed Carbon	43.09	27.54
Total	100	100
Ultimate Analysis	Dry Basis, %	As Received, %
Carbon	61.88	39.55
Hydrogen	4.29	2.74
Nitrogen	0.98	0.63
Sulfur	0.98	0.63
Chlorine ²	18 ppmW	12 ppmW
Ash	15.43	9.86
Moisture	0	36.08
Oxygen	16.44	10.51
Total	100	100
Heating Value	Dry Basis	As Received
HHV, kJ/kg	24,253	15,391
HHV, Btu/lb	10,427	6,617
LHV, kJ/kg	23,334	14,803
LHV, Btu/lb	10,032	6,364
Trace Components		
Mercury, ppm		0.116

² The Cl content is taken from paper titled, "Comparison of Sorbents and Furnace Additives for Mercury Control in Low Rank Fuel Combustion Systems," by C. R. Crocker, S. A. Benson, M.I J. Holmes, Y. Zhuang, J. H. Pavlish, K. C. Galbreath [Prepr. Pap.-Am. Chem. Soc., Div. Fuel Chem. 2004, 49 (1), 289]

3.3 Carbon Dioxide Product Specification

The specifications of the CO₂ product are based on the typical purity obtained by the Selexol™ cold gas cleanup process which was used in the previously referenced DOE/NETL report without any further purification. The Argon content in the CO₂ stream coming off the TDA's PSA unit is similar to what is typically obtained from a Selexol™ unit, i.e., without any further purification. This eliminated the need for cryogenic distillation in the CO₂ purification process and instead a catalytic combustor to burn any residual syngas present in the CO₂ stream with oxygen from the air separation unit (ASU) was utilized. Table 3-3 summarizes the CO₂ specifications used for this analysis.

Table 3-3: CO₂ Pipeline Specification

Parameter Units	Parameter Value
Inlet Pressure MPa (psia)	15.3 (2,215)
Outlet Pressure MPa (psia)	10.4 (1,515)
Inlet Temperature °C (°F)	35 (95)
CO ₂ Concentration, mole %	> 95
N ₂ Concentration	not limited
O ₂ Concentration ppmv	< 40
Ar Concentration	not limited
H ₂ O Concentration ppmv	< 150

3.4 Property Packages

The performance of the plant was estimated using the Aspen Plus Simulator software, and the following property packages were used to model the cycle:

- PR-BM (Peng-Robinson equation of state with Boston-Mathias modifications) for most plant section systems except as follows
- ElecNRTL (Electrolyte Non-random Two Liquid model, also known as the Chen electrolyte model, formulated for modeling aqueous electrolytes) for sour water systems
- STEAM-TA (ASME 1967 Steam Table Corrections) for the water and steam.

3.5 Process Descriptions

3.5.1 Cold Gas Cleanup

The IGCC plant employing the cold gas cleanup and CO₂ capture technology depicted in Figure 3-1 consists of the following plant subsystems. The major stream data for the subbituminous and the lignite are presented in Tables 3-1 and 3-2 for a coal feed rate of 292,295 kg/h on an

“as received” basis. Note that this flow rate of coal does not fully load the two gas turbines and the corresponding stream data should be scaled to fully load the two gas turbines. This coal flow rate however is held the same as in the corresponding Warm Gas Cleanup cases and allows a more direct comparison of the various plant streams between the two subbituminous cases and between the two lignite cases (but not for cross comparison between the two different types of coals).

- Air Separation Unit (ASU)
- Coal Feed Preparation
- Gasification (based on Phillips 66 technology)
- High Temperature Syngas Cooling and Scrubbing
- Sour Shifting and Cold Gas Heat Recovery
- Syngas Desulfurization and Decarbonization using a two-stage Selexol™ process
- Claus Sulfur Recovery and Tail Gas Hydrogenation followed by Recycle to the Gasifier
- CO₂ Dehydration and Pressurization (the pressurization scheme was modified to include first compression to a pressure such that the CO₂ stream forms a liquid when cooled against the cooling water, followed by pumping to the final pressure in order to reduce the parasitic load of pressurization)
- Gas Turbine (based on GE F class technology type)
- Heat Recovery Steam Generator Unit
- Reheat Steam Cycle

The plant also has the necessary utilities (e.g. cooling water supply, make-up water treatment, plant and instrument air) to support the process units.

Detailed process description of this type of plant may be found in the previously referenced DOE/NETL report.

3.5.2 Warm Gas Cleanup

The IGCC plant employing the sorbent CO₂ capture consists of the following plant subsystems:

- Air Separation Unit (ASU)
- Coal Feed Preparation
- Gasification (based on Phillips 66 technology)
- High Temperature Syngas Cooling and Scrubbing
- Warm Gas Cleanup similar to RTI's process including Acid (H₂SO₄) Unit
- First Stage of Shifting
- Combined Shifting and Regenerable Sorbent CO₂ Capture (based on TDA technology)
- CO₂ Purification and Pressurization
- Gas Turbine (based on GE F class technology type)
- Heat Recovery Steam Generator Unit
- Reheat Steam Cycle

The overall configuration of the IGCC plant with TDA's combined shift and high temperature PSA-based CO₂ capture system is shown in Figure 3-2 while the major stream data for the subbituminous and the lignite cases are presented in Tables 3-3 and 3-4. Plant subsystems that are different from the Cold Gas Cleanup case are described in the following.

As in the cold gas cleanup case, 7% of the raw syngas exiting the scrubber is compressed and recycled back to the gasifier system as quench gas.

Remainder of the scrubbed gas is preheated to a temperature of 260°C in a feed/effluent exchanger and supplied to a warm gas cleanup unit similar to RTI's process for removal of sulfur compounds utilizing a zinc titanate adsorbent in a fluidized bed. The performance of this unit as well as the production of H₂SO₄ from the SO₂ in the regenerator off-gas was developed utilizing information available in the public domain. The regenerator off-gas after particulate removal is depressurized by expansion in a power recovery turbine before feeding it to the H₂SO₄ unit. The on-site ASU provides the small amount of O₂ as required by the H₂SO₄ unit in addition to supplying oxygen to the gasifier and the catalytic combustor used for CO₂ purification (combust the residuals amounts of H₂, CO and CH₄). The hot syngas leaving the desulfurizer is cooled (to a temperature of 224°C for the subbituminous case and 231°C for the lignite case) in the feed/effluent exchanger where the desulfurizer feed gas is preheated.

The clean gas is then treated in a shift reactor similar to the 1st stage reactor of the Cold Gas Cleanup case. The effluent is cooled by generating intermediate pressure (IP) and medium pressure (MP) steam. The partially shifted syngas leaving this shift reactor (at a temperature of 210°C for the subbituminous case and 232°C for the lignite case) is combined with recycle gas from the downstream TDA's combined shift and PSA unit and then fed to this TDA's unit for further shifting and simultaneously decarbonizing the syngas before it is combusted in the gas turbines as depicted in Figure 3-3. About 98% of the syngas enters this simultaneous shifting and decarbonizing unit to result in an overall carbon capture of 90%. Remainder of the syngas is sent directly to the gas turbine bypassing TDA's CO₂ capture system. Regeneration is accomplished utilizing steam at a desorption pressure of 10 barA. Two streams are regenerated, one consisting of "raw CO₂," a mixture of CO₂, steam and small amounts of residual syngas at the desorption pressure and the other "recycle gas," with significant amounts of other syngas components (mainly H₂) at a lower pressure of 9.38 bar for recycle to the combined shift and CO₂ separation unit. The raw CO₂ is cooled in a series of heat exchangers while generating low pressure (LP) steam, vacuum condensate/makeup BFW heating and finally trim cooled against cooling water before it is compressed, preheated in a feed/effluent exchanger and then fed to a catalytic (noble meta containing) combustor along with O₂ to oxidize the small amounts of combustibles present in the raw CO₂ stream. The effluent from this combustor after generating HP steam is cooled in the feed/effluent exchanger. This is followed by vacuum condensate/makeup BFW heating and finally trim cooled against cooling water. It is then further compressed to a pressure such that the CO₂ stream forms a liquid when cooled against the cooling water. This liquid CO₂ stream leaving the cooling water exchanger is then pumped to the final pressure (note that a similar scheme was used in the Cold Gas Cleanup case to maintain consistency).

The decarbonized syngas leaving the combined shift and CO₂ separation (adsorption) unit (at a temperature of 208°C in the case of the subbituminous coal and 221°C in the case of the lignite) with its accompanying unreacted steam is supplied to the gas turbines. In the case of the subbituminous coal, additional diluent in the form of N₂ (pressurized, humidified and preheated) from the ASU is required, the amount of N₂ added is significantly lower than that in the corresponding Cold Gas Cleanup case due to the large amount of water vapor present in the syngas. The combined cycle design is similar to the design in the Cold Gas Cleanup case consisting of a reheat steam cycle.

Figure 3-1: Block flow diagram for IGCC plant with cold gas CO₂ capture system

Figure 3-2: Block flow diagram for IGCC plant with TDA’s combined shift and high-temperature PSA-based CO₂ capture system

Figure 3-3: Block flow diagram of TDA's combined shift and high temperature PSA-based CO₂ capture system along with the CO₂ purification and compression system

Table 3-1
Stream Data
Cold Gas Cleanup – Subbituminous Coal (292,295 kg/h as received)

STREAM NO.	1	2	3	4	5	6	7	8	9	9A	10	11	12
Temperature, C	15	91	149	79	232	218	58	60	206	398	38	345	226
Pressure, bar	1.01	59.64	66.19	70.67	7.93	30.52	3.10	1.01	48.72	51.02	43.89	7.31	2.10
Solids, kg/hr	292345	0	292345	0	0	0	5587	19666	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	0.001	0	1	1	1	1	1
kmol/hr (w/o Solids)	0	0.01	6162	5917	52	15975	353	0	35334	1566	26008	3013	386
kg/hr (w/o Solids)	0	0.292	111015	190420	1673	448307	6373	0	730087	28216	555517	54273	14140
Mole Frac (w/o Solids)													
O2	0	0.005	0	0.95	0.95	0.005	0	0	0	0	0	0	0
N2	0	0.992	0	0.018	0.018	0.992	0	0	0.005	0	0.007	0	0.001
AR	0	0.002	0	0.032	0.032	0.002	0	0	0.006	0	0.007	0	0.002
H2	0	0	0	0	0	0	0	0	0.213	0	0.518	0	0.112
CO	0	0	0	0	0	0	0	0	0.206	0	0.012	0	0.004
CO2	0	0	0	0	0	0	0	0	0.146	0	0.434	0	0.675
H2O	0	0	1	0	0	0	0.998	0	0.406	1	0.001	1	0.021
CH4	0	0	0	0	0	0	0	0	0.015	0	0.019	0	0.01
H2S	0	0	0	0	0	0	0	0	0.002	0	0.003	0	0.175
HCl	0	0	0	0	0	0	0.002	0	0	0	0	0	0

Table 3-1 (Cont'd)
Stream Data
Cold Gas Cleanup – Subbituminous Coal (292,295 kg/h as received)

STREAM NO.	13	14	15	16	17	18	19	20	21	22	23
Temperature, C	174	139	14	11	11	32	21	218	6	564	154
Pressure, bar	1.45	63.40	10.93	17.24	20.62	152.70	41.44	40.75	0.90	0.93	0.87
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	1	1	0.989	0	1	1	1	1	1
kmol/hr (w/o Solids)	33	305	5528	3938	1404	10855	15041	15041	107876	132034	132034
kg/hr (w/o Solids)	2125	11971	243306	173326	59236	475575	77258	77258	3117040	3642610	3642610
Mole Frac (w/o Solids)											
O2	0	0	0	0	0	0	0	0	0.208	0.112	0.112
N2	0	0.016	0	0	0	0	0.012	0.012	0.776	0.755	0.755
AR	0	0.008	0	0	0.001	0	0.013	0.013	0.009	0.009	0.009
H2	0	0.093	0	0	0.03	0.004	0.891	0.891	0	0	0
CO	0	0.008	0	0	0.003	0	0.021	0.021	0	0	0
CO2	0	0.857	1	1	0.947	0.995	0.032	0.032	0	0.01	0.01
H2O	0	0.004	0	0	0.012	0	0	0	0.006	0.114	0.114
CH4	0	0.009	0	0	0.007	0.001	0.031	0.031	0	0	0
H2S	0	0.004	0	0	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0	0	0

Table 3-2
Stream Data
Cold Gas Cleanup – Lignite Coal (292,295 kg/h as received)

STREAM NO.	1	2	3	4	5	6	7	8	9	9A	10	11	12
Temperature, C	15	94	149	72	232	215	58	60	215	265	38	331	226
Pressure, bar	1.01	59.64	66.19	71.69	7.93	30.52	3.10	1.01	48.72	51.02	43.89	7.31	2.10
Solids, kg/hr	292345	0	292345	0	0	0	6712	23625	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	0	0	1	0.678	1	1	1
kmol/hr (w/o Solids)	0	0.01	5702	5295	47	19598	3958	0	31290	0	19225	2421	306
kg/hr (w/o Solids)	0	0.292	102722	170419	1503	549977	71314	0	662319	3	438058	43608	11397
Mole Frac (w/o Solids)													
O2	0	0.005	0	0.95	0.95	0.005	0	0	0	0	0	0	0
N2	0	0.992	0	0.018	0.018	0.992	0	0	0.005	0	0.008	0	0.001
AR	0	0.002	0	0.032	0.032	0.002	0	0	0.006	0	0.009	0	0.003
H2	0	0	0	0	0	0	0	0	0.181	0	0.484	0	0.097
CO	0	0	0	0	0	0	0	0	0.143	0	0.006	0	0.002
CO2	0	0	0	0	0	0	0	0	0.17	0	0.468	0	0.678
H2O	0	0	1	0	0	0	1	0	0.479	1	0.001	1	0.019
CH4	0	0	0	0	0	0	0	0	0.013	0	0.019	0	0.01
H2S	0	0	0	0	0	0	0	0	0.002	0	0.003	0	0.189

Table 3-2 (Cont'd)
Stream Data
Cold Gas Cleanup – Lignite Coal (292,295 kg/h as received)

STREAM NO.	13	14	15	16	17	18	19	20	21	22	23
Temperature, C	174	138	13	11	11	31	20	215	4	561	152
Pressure, bar	1.45	63.40	10.93	17.24	20.62	152.70	41.44	40.75	0.95	0.99	0.93
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	1	1	0.99	0	1	1	1	1	1
kmol/hr (w/o Solids)	29	246	4362	3109	1103	8562	10574	10574	64597	90074	90074
kg/hr (w/o Solids)	1829	9773	191983	136818	46758	375347	60627	60627	1866670	2477280	2477280
Mole Frac (w/o Solids)											
O2	0	0	0	0	0	0	0	0	0.208	0.09	0.09
N2	0	0.024	0	0	0.001	0	0.015	0.015	0.776	0.774	0.774
AR	0	0.01	0	0	0.001	0	0.016	0.016	0.009	0.009	0.009
H2	0	0.081	0	0	0.026	0.003	0.877	0.877	0	0	0
CO	0	0.006	0	0	0.001	0	0.011	0.011	0	0	0
CO2	0	0.861	1	1	0.953	0.995	0.046	0.046	0	0.011	0.011
H2O	0	0.004	0	0	0.011	0	0	0	0.006	0.115	0.115
CH4	0	0.009	0	0	0.007	0.001	0.034	0.034	0	0	0
H2S	0	0.005	0	0	0	0	0	0	0	0	0

Table 3-3
Stream Data
Warm Gas Cleanup – Subbituminous Coal (292,295 kg/h as received)

STREAM NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Temperature, C	15	86	149	92	59	32	288	145	59	60	205	15	334	6	141	20	43	210
Pressure, bar	1.01	51.37	66.19	70.67	41.20	8.62	30.52	20.50	3.10	1.01	48.72	1.01	2.07	0.90	8.00	1.01	1.01	44.16
Solids, kg/hr	292345	0	292345	0	0	0	0	0	5587	19666	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	1	1	0.013	0	1	1	1	1	0	0	1	1
kmol/hr (w/o Solids)	0	0.01	6162	5906	108	40	5215	169	46	0	34840	506	576	201	64	66	718	32783
kg/hr (w/o Solids)	0	0.292	111015	190083	3028	1290	133873	5454	835	0	720954	14607	18612	5820	1159	6490	20419	676307
Mole Frac (w/o Solids)																		
O2	0	0.005	0	0.95	0.005	0.95	0.004	0.95	0	0	0	0.208	0.011	0.208	0	0	0.074	0
N2	0	0.992	0	0.018	0.992	0.018	0.756	0.018	0	0	0.005	0.772	0.864	0.776	0	0	0.913	0.005
AR	0	0.002	0	0.032	0.002	0.032	0.002	0.032	0	0	0.006	0.009	0.009	0.009	0	0	0.011	0.006
H2	0	0	0	0	0	0	0	0	0	0	0.216	0	0	0	0	0	0	0.381
CO	0	0	0	0	0	0	0	0	0	0	0.209	0	0	0	0	0	0	0.04
CO2	0	0	0	0	0	0	0	0	0	0	0.148	0	0	0	0	0	0.001	0.314
H2O	0	0	1	0	0	0	0.238	0	0.987	0	0.398	0.011	0.001	0.006	1	0.005	0.001	0.24
CH4	0	0	0	0	0	0	0	0	0	0	0.015	0	0	0	0	0	0	0.015
H2S	0	0	0	0	0	0	0	0	0	0	0.002	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0.013	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0.115	0	0	0	0	0
H2SO4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.995	0	0

Table 3-3 (Cont'd)
Stream Data
Warm Gas Cleanup – Subbituminous Coal (292,295 kg/h as received)

STREAM NO.	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
Temperature, C	207	180	39	208	6	577	153	228	209	26	92	288	430	136	26	57	20
Pressure, bar	10.34	10.00	152.70	42.57	0.90	0.93	0.87	10.11	44.16	9.38	20.00	19.79	19.10	18.55	17.79	60.00	59.66
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0
kmol/hr (w/o Solids)	12591	19751	10794	25309	102387	126158	126158	3191	34944	11099	11099	11099	11128	11128	10794	10794	10794
kg/hr (w/o Solids)	226835	631332	474904	266134	2958430	3358440	3358440	100075	755949	475459	475459	475459	480913	480913	474904	474904	474904
Mole Frac (w/o Solids)																	
O2	0	0	0	0	0.208	0.108	0.108	0	0	0	0	0	0	0	0	0	0
N2	0	0	0.001	0.007	0.776	0.662	0.662	0.003	0.005	0	0	0	0.001	0.001	0.001	0.001	0.001
AR	0	0	0.001	0.007	0.009	0.009	0.009	0.003	0.006	0	0	0	0.001	0.001	0.001	0.001	0.001
H2	0	0.014	0	0.521	0	0	0	0.224	0.398	0.025	0.025	0.025	0	0	0	0	0
CO	0	0	0	0.013	0	0	0	0.005	0.009	0.001	0.001	0.001	0	0	0	0	0
CO2	0	0.545	0.999	0.02	0	0.011	0.011	0.646	0.375	0.97	0.97	0.97	0.969	0.969	0.999	0.999	0.999
H2O	1	0.44	0	0.413	0.006	0.21	0.21	0.111	0.193	0.003	0.003	0.003	0.03	0.03	0	0	0
CH4	0	0.001	0	0.019	0	0	0	0.008	0.014	0.001	0.001	0.001	0	0	0	0	0
H2S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HCl	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 3-4
Stream Data
Warm Gas Cleanup – Lignite Coal (292,295 kg/h as received)

STREAM NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Temperature, C	15	93	149	95	60	28	196	518	58	60	213	4	334	4	141	20	43	232
Pressure, bar	1.01	51.37	66.19	70.67	41.20	1.03	30.52	20.50	3.10	1.01	48.72	0.95	2.07	0.95	8.00	1.01	1.01	44.16
Solids, kg/hr	292345	0	292345	0	0	0	0	0	6712	23625	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)		1	0	1	1	1	1	1	0	0	1	1	1	1	0	0	1	1
kmol/hr (w/o Solids)	0	0	5702	5283	92	34	0	100	3956	0	30318	433	494	173	55	58	619	28193
kg/hr (w/o Solids)	0	0	102722	170031	2574	1106	0	3211	71278	0	644934	12499	15946	4987	995	5602	17644	598842
Mole Frac (w/o Solids)																		
O2	0	0.005	0	0.95	0.005	0.95	0.005	0.95	0	0	0	0.208	0.011	0.208	0	0	0.07	0
N2	0	0.992	0	0.018	0.992	0.018	0.992	0.018	0	0	0.005	0.776	0.864	0.776	0	0	0.908	0.005
AR	0	0.002	0	0.032	0.002	0.032	0.002	0.032	0	0	0.006	0.009	0.009	0.009	0	0	0.011	0.006
H2	0	0	0	0	0	0	0	0	0	0	0.184	0	0	0	0	0	0	0.315
CO	0	0	0	0	0	0	0	0	0	0	0.149	0	0	0	0	0	0	0.018
CO2	0	0	0	0	0	0	0	0	0	0	0.174	0	0	0	0	0	0.007	0.305
H2O	0	0	1	0	0	0	0	0	1	0	0.465	0.006	0.001	0.006	1	0.018	0.003	0.336
CH4	0	0	0	0	0	0	0	0	0	0	0.014	0	0	0	0	0	0	0.014
H2S	0	0	0	0	0	0	0	0	0	0	0.002	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0.115	0	0	0	0	0
H2SO4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.982	0	0

Table 3-4 (Cont'd)
Stream Data
Warm Gas Cleanup – Lignite Coal (292,295 kg/h as received)

STREAM NO.	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
Temperature, C	205	201	38	221	4	580	152	227	225	26	93	288	398	136	27	56	19
Pressure, bar	10.34	10.00	152.70	42.57	0.95	0.99	0.93	10.11	44.16	9.25	20.00	19.79	19.10	18.55	17.79	60.00	59.66
Solids, kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Vapor Frac (w/o Solids)	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0
kmol/hr (w/o Solids)	10375	15729	8487	22360	68798	86538	86538	2691	29853	8671	8671	8671	8689	8689	8487	8487	8487
kg/hr (w/o Solids)	186916	500997	373410	276106	1988050	2264150	2264150	81967	660444	373843	373843	373843	377053	377053	373410	373410	373410
Mole Frac (w/o Solids)																	
O2	0	0	0	0	0.208	0.103	0.103	0	0	0	0	0	0	0	0	0	0
N2	0	0	0.001	0.007	0.776	0.619	0.619	0.003	0.005	0	0	0	0.001	0.001	0.001	0.001	0.001
AR	0	0	0.001	0.007	0.009	0.009	0.009	0.004	0.006	0	0	0	0.001	0.001	0.001	0.001	0.001
H2	0	0.01	0	0.406	0	0	0	0.197	0.322	0.018	0.018	0.018	0	0	0	0	0
CO	0	0	0	0.007	0	0	0	0.003	0.005	0	0	0	0	0	0	0	0
CO2	0	0.538	0.999	0.022	0	0.012	0.012	0.595	0.348	0.977	0.977	0.977	0.976	0.976	0.999	0.999	0.999
H2O	1	0.451	0	0.534	0.006	0.257	0.257	0.19	0.3	0.003	0.003	0.003	0.023	0.023	0	0	0
CH4	0	0	0	0.017	0	0	0	0.008	0.013	0.001	0.001	0.001	0	0	0	0	0
H2S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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4.0 Results and Discussion

The plant performance of the four cases is summarized in Tables 4-1 and 4-2 with the flow rates scaled to fully load the two gas turbines. It should be noted that the performance of the gas turbine for each of these cases was estimated by UCI and it is recommended that in a more detailed phase of this development program, gas turbine vendors be contacted for providing performance data. The effective LHV of the syngas provided to the gas turbines was held constant for each of the cases by adjusting the amount of diluent, i.e., moisture introduced into the syngas by the humidification operation in the case of cold gas cleanup, and amount of humidified nitrogen (supplied by the ASU) in the case of the subbituminous coal warm gas cleanup case while the lignite warm gas cleanup case required no additional diluent in the form of N₂. The need for the additional diluent in the form of humidified nitrogen in the subbituminous coal warm gas cleanup case limited its efficiency gain over the corresponding cold gas cleanup case. The molar ratio of moisture to N₂ is significantly higher for the warm gas cleanup case and since H₂O has a much higher specific heat than N₂, it may be expected that the NO_x emission for this case will be significantly lower. We also carried out comparison of the warm gas cleanup cases against the cold gas cleanup cases on the basis of same coal feed rate of 292,295 kg/h (as received) and the performance results are summarized in Table 4-3 and Table 4-4 for the two types of coal.

The plant cost and the levelized cost of electricity estimates for the Cold Gas Cleanup Cases and the Warm gas Cleanup Cases are presented in Tables 4-5 through 4-8 with the flow rates scaled to fully load the two gas turbines.

4.1 Subbituminous Coal Cases

The calculated net thermal efficiency of the Warm Gas Cleanup Case is significantly higher at 32.90% versus 31.35% (on a coal HHV basis) for the Cold Gas Cleanup Case.

On a constant coal throughput basis, the cold gas capture case produced higher total power than warm gas capture. This is due to more power being generated in the gas turbine for the cold gas cleanup case. Water vapor is the major diluent present in the syngas entering gas turbine in the warm gas cleanup case while N₂ from ASU is the major diluent present in the syngas entering the gas turbine in the cold gas cleanup case. Less amount of water vapor is required to achieve the same level of NO_x emissions as with N₂. This reduces the gas turbine output for the warm gas cleanup case when expressed on a unit coal flow basis.

However, the net power produced is higher for the warm gas cleanup with lower auxiliary loads (134,862 kWe) in the case of warm gas cleanup with TDA's combined shift and CO₂ capture system compared to cold gas cleanup (181,112 kWe) with SelexolTM providing a net difference in auxiliary load of 46.25 MWe. There are two major subsystems that result in this reduction in auxiliary load for the warm gas cleanup case: the ASU and the CO₂ capture and sulfur removal system.

In the case of the ASU the power consumption (air, O₂ and N₂ compression + auxiliaries) for cold gas cleanup case is very high (112.41 MWe) compared to warm gas cleanup case (82.30 MWe) (a net difference of 30.11 MWe). The ASU was modeled as comprising a low pressure

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(LP) ASU and an elevated pressure (EP) ASU for both the cases. The relative size of these two units is set by the amount of nitrogen required for gas turbine injection to minimize compression of air. The warm gas cleanup case requires less nitrogen for gas turbine and thus the size of the EP ASU unit is smaller (while that of the LP ASU is larger) when compared to cold gas cleanup case. Hence the auxiliary load for air compression is higher for cold gas cleanup case. Also the diluent N₂ supplied by the ASU to the gas turbine requires a significant amount of compression (from the pressure leaving the elevated pressure cold box to that required by the gas turbine). Hence the auxiliary load for the nitrogen compressor is higher for cold gas capture. However, the auxiliary load for oxygen compressor is higher for warm gas cleanup case since more oxygen from the LP ASU needs to be compressed for use in the gasifier and the catalytic combustor.

The auxiliary load for CO₂ separation, purification and compression and sulfur removal for the warm gas cleanup case with TDA's combined shift and high temperature PSA system is significantly lower at 26.03 MWe compared to 40.38 MWe for cold gas cleanup with Selexol™ (a net difference of 14.35 MWe).

The above results indicate that warm gas cleanup technology coupled with the combined shift and CO₂ adsorption process being developed by TDA can make a substantial improvement in the IGCC plant thermal performance designed for approaching near zero emissions, i.e., to include CO₂ capture.

The plant cost for the Warm gas Cleanup Case is \$2824/kW while that for the Cold Gas Case is \$2993/kW, or a decrease of about 6% over the Cold Gas Cleanup Case. The levelized cost of electricity with transport, storage and monitoring (TS&M) costs for the CO₂ included is \$100.1/MWh for the Warm gas Cleanup Case while that for the Cold Gas Case is \$105.3/MWh, or a decrease of about 5% over the Cold Gas Cleanup Case.

4.2 Lignite Coal Cases

The calculated net thermal efficiency of the Warm Gas Cleanup Case is significantly higher at 30.42% versus 28.28% (on a coal HHV basis) for the Cold Gas Cleanup Case.

On a constant coal throughput basis, the cold gas capture case produced higher total power than warm gas capture. This is due to more power being generated in the gas turbine for the cold gas cleanup case. Water vapor is the major diluent present in the syngas entering gas turbine in the warm gas cleanup case while N₂ from ASU is the major diluent present in the syngas entering the gas turbine in the cold gas cleanup case. Less amount of water vapor is required to achieve the same level of NO_x emissions as with N₂. This reduces the gas turbine output for the warm gas cleanup case when expressed on a unit coal flow basis.

However, the net power produced is higher for the warm gas cleanup with lower auxiliary loads (158,416 kWe) in the case of warm gas cleanup with TDA's combined shift and CO₂ capture system compared to cold gas cleanup (241,194 kWe) with Selexol™ providing a net difference in auxiliary load of 82.78 MWe. There are two major subsystems that result in this reduction in auxiliary load for the warm gas cleanup case: the ASU and the CO₂ capture and sulfur removal system.

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In the case of the ASU the power consumption for cold gas cleanup case is very high (161.70 MWe) compared to warm gas cleanup case (84.47 MWe) (a net difference of 77.23 MWe). The ASU was modeled as comprising a low pressure (LP) ASU and an elevated pressure (EP) ASU for both the cases. The relative size of these two units is set by the amount of nitrogen required for gas turbine injection to minimize compression of air. The warm gas cleanup case requires less nitrogen for gas turbine and thus the size of the EP ASU unit is smaller (while that of the LP ASU is larger) when compared to cold gas cleanup case. Hence the auxiliary load for air compression is higher for cold gas cleanup case. Also the diluent N₂ supplied by the ASU to the gas turbine requires a significant amount of compression (from the pressure leaving the elevated pressure cold box to that required by the gas turbine). Hence the auxiliary load for the nitrogen compressor is higher for cold gas capture. However, the auxiliary load for oxygen compressor is higher for warm gas cleanup case since more oxygen from the LP ASU needs to be compressed for use in the gasifier and the catalytic combustor.

The auxiliary load for CO₂ separation, purification and compression and sulfur removal for the warm gas cleanup case with TDA's combined shift and high temperature PSA system is significantly lower at 28.28 MWe compared to 45.09 MWe for cold gas cleanup with SelexolTM (a net difference of 16.81 MWe).

The above results indicate that warm gas cleanup technology coupled with the combined shift and CO₂ adsorption process being developed by TDA can make a substantial improvement in the IGCC plant thermal performance designed for approaching near zero emissions, i.e., to include CO₂ capture.

The plant cost for the Warm gas Cleanup Case is \$2990/kW while that for the Cold Gas Case is \$3348/kW, or a decrease of as much as 11% over the Cold Gas Cleanup Case. The levelized cost of electricity with transport, storage and monitoring (TS&M) costs for the CO₂ included is \$105.8/MWh for the Warm gas Cleanup Case while that for the Cold Gas Case is \$117.0/MWh, or a decrease of about 10% over the Cold Gas Cleanup Case.

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**Table 4-1
Overall Plant Performance Summary
Subbituminous Coal Cases – Fully Loaded GTs**

	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	Kwe	430,900	430,900
STEAM TURBINE POWER	Kwe	262,055	254,311
TOTAL GROSS POWER	Kwe	692,955	685,211
TOTAL AUXILIARY CONSUMPTION	Kwe	181,112	134,862
NET POWER OUTPUT	Kwe	511,843	550,349
AUXILIARY LOAD SUMMARY			
COAL HANDLING	Kwe	599	614
COAL MILLING	Kwe	3,036	3,110
COAL SLURRY PUMPS	Kwe	658	674
SLAG HANDLING & DEWATERING	Kwe	1,499	1,534
AIR SEPARATION UNIT AUXILIARIES	Kwe	1,162	1,219
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	Kwe	65,733	49,412
OXYGEN COMPRESSOR	Kwe	15,579	23,681
NITROGEN COMPRESSOR	Kwe	29,941	7,984
SYNGAS RECYCLE COMPRESSOR	Kwe	520	532
TAIL GAS RECYCLE COMPRESSOR	Kwe	1,584	-
CO2 PURIFICATION & COMPRESSION	Kwe	20,345	25,499
BOILER FEEDWATER & DEMIN PUMPS	Kwe	4,459	4,891
VACUUM CONDENSATE PUMP	Kwe	283	290
PROCESS CONDENSATE & SWS SYSTEMS	Kwe	235	580
BFW CIRCULATING PUMPS	Kwe	23	97
COOLING WATER CIRCULATING PUMPS	Kwe	3,411	2,965
COOLING TOWER + AIR COOLER FANS	Kwe	5,277	4,469
SCRUBBER PUMPS	Kwe	95	98
SELEXOL UNIT	Kwe	19,957	-
DESULFURIZER UNIT	Kwe	-	2,068
GAS TURBINE AUXILIARIES	Kwe	929	929
STEAM TURBINE AUXILIARIES	Kwe	114	111
CLAUS & TAIL GAS TREATING AUXILIARIES	Kwe	79	-
H2SO4 UNIT	Kwe	-	-1,535
MISCELLANEOUS BALANCE OF PLANT	Kwe	3,028	3,102
TRANSFORMER LOSSES	Kwe	2,567	2,538
NET PLANT EFFICIENCY, HHV	%	31.35	32.90
NET HEAT RATE	KJ/KWH	11,485	10,942
	BTU/KWH	10,885	10,371
CONDENSER COOLING DUTYNET	10^6 KJ/H	735	612
	10^6 BTU/H	696	580
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	295,046	302,251
	LB/H	650,575	666,462
THERMAL INPUT	KWT HHV	1,632,443	1,672,307
RAW WATER USAGE	M^3/MIN	14.42	15.96
	GPM	3,809	4,216
CARBON CAPTURED	%	90	90

**Table 4-2
Overall Plant Performance Summary
Lignite Coal Cases – Fully Loaded GTs**

CASE DESIGNATION	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	kWe	456,600	456,600
STEAM TURBINE POWER	kWe	289,856	299,807
TOTAL GROSS POWER	kWe	746,456	756,407
TOTAL AUXILIARY CONSUMPTION	kWe	241,194	158,416
NET POWER OUTPUT	kWe	505,262	597,992
AUXILIARY LOAD SUMMARY			
COAL HANDLING	kWe	848	934
COAL MILLING	kWe	4,300	4,731
COAL SLURRY PUMPS	kWe	859	946
SLAG HANDLING & DEWATERING	kWe	2,150	2,366
AIR SEPARATION UNIT AUXILIARIES	kWe	1,472	1,643
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	kWe	92,751	55,572
OXYGEN COMPRESSOR	kWe	15,084	35,424
NITROGEN COMPRESSOR	kWe	52,395	310
SYNGAS RECYCLE COMPRESSOR	kWe	559	614
TAIL GAS RECYCLE COMPRESSOR	kWe	1,808	-
CO2 PURIFICATION & COMPRESSION	kWe	22,670	30,410
BOILER FEEDWATER & DEMIN PUMPS	kWe	4,943	5,971
VACUUM CONDENSATE PUMP	kWe	304	334
PROCESS CONDENSATE & SWS SYSTEMS	kWe	366	1,018
HUMIDIFIER & BFW CIRCULATING PUMPS	kWe	28	152
COOLING WATER CIRCULATING PUMPS	kWe	4,175	3,579
COOLING TOWER + AIR COOLER FANS	kWe	5,758	4,923
SCRUBBER PUMPS	kWe	135	149
SELEXOL UNIT	kWe	22,328	-
DESULFURIZER UNIT	kWe	-	2,718
GAS TURBINE AUXILIARIES	kWe	984	984
STEAM TURBINE AUXILIARIES	kWe	126	130
CLAUS & TAIL GAS TREATING AUXILIARIES	kWe	96	-
H2SO4 UNIT	kWe	-	-2,012
MISCELLANEOUS BALANCE OF PLANT	kWe	4,289	4,719
TRANSFORMER LOSSES	kWe	2,765	2,802
NET PLANT EFFICIENCY, HHV	%	28.28	30.42
NET HEAT RATE	KJ/KWH	12,731	11,836
	BTU/KWH	12,067	11,219
CONDENSER COOLING DUTYNET POWER	10^6 KJ/H	816	696
	10^6 BTU/H	773	660
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	417,873	459,799
	LB/H	921,411	1,013,856
THERMAL INPUT	KWT HHV	1,786,398	1,965,628
RAW WATER USAGE	M^3/MIN	17.22	21.07
	GPM	4,550	5,567
CARBON CAPTURED	%	90	90

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**Table 4-3
Overall Plant Performance Summary
Subbituminous Coal Cases – Coal feed rate of 292,295 kg/h (as received)**

	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	Kwe	426,882	416,707
STEAM TURBINE POWER	Kwe	259,612	245,935
TOTAL GROSS POWER	Kwe	686,494	662,642
TOTAL AUXILIARY CONSUMPTION	Kwe	179,424	130,420
NET POWER OUTPUT	Kwe	507,071	532,222
AUXILIARY LOAD SUMMARY			
COAL HANDLING	Kwe	593	593
COAL MILLING	Kwe	3,008	3,008
COAL SLURRY PUMPS	Kwe	652	652
SLAG HANDLING & DEWATERING	Kwe	1,485	1,484
AIR SEPARATION UNIT AUXILIARIES	Kwe	1,151	1,179
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	Kwe	65,121	47,785
OXYGEN COMPRESSOR	Kwe	15,433	22,901
NITROGEN COMPRESSOR	Kwe	29,662	7,721
SYNGAS RECYCLE COMPRESSOR	Kwe	515	515
TAIL GAS RECYCLE COMPRESSOR	Kwe	1,569	-
CO2 PURIFICATION & COMPRESSION	Kwe	20,155	24,659
BOILER FEEDWATER & DEMIN PUMPS	Kwe	4,417	4,730
VACUUM CONDENSATE PUMP	Kwe	280	280
PROCESS CONDENSATE & SWS SYSTEMS	Kwe	233	561
BFW CIRCULATING PUMPS	Kwe	23	94
COOLING WATER CIRCULATING PUMPS	Kwe	3,379	2,867
COOLING TOWER + AIR COOLER FANS	Kwe	5,227	4,322
SCRUBBER PUMPS	Kwe	94	94
SELEXOL UNIT	Kwe	19,771	-
DESULFURIZER UNIT	Kwe	-	1,999
GAS TURBINE AUXILIARIES	Kwe	920	898
STEAM TURBINE AUXILIARIES	Kwe	113	107
CLAUS & TAIL GAS TREATING AUXILIARIES	Kwe	78	-
H2SO4 UNIT	Kwe	-	-1,485
MISCELLANEOUS BALANCE OF PLANT	Kwe	3,000	3,000
TRANSFORMER LOSSES	Kwe	2,543	2,454
NET PLANT EFFICIENCY, HHV	%	31.35	32.90
NET HEAT RATE	KJ/KWH	11,485	10,942
	BTU/KWH	10,885	10,371
CONDENSER COOLING DUTYNET POWER	10^6 KJ/H	728	592
	10^6 BTU/H	690	561
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	292,295	292,295
	LB/H	644,510	644,510
THERMAL INPUT	KWT HHV	1,617,223	1,617,224
RAW WATER USAGE	M^3/MIN	14.28	15.43
	GPM	3,774	4,077
CARBON CAPTURED	%	90	90

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**Table 4-4
Overall Plant Performance Summary
Lignite Coal Cases – Coal feed rate of 292,295 kg/h (as received)**

CASE DESIGNATION	UNITS	COLD GAS CLEANUP	WARM GAS CLEANUP
GAS TURBINE POWER	kWe	319,383	290,262
STEAM TURBINE POWER	kWe	202,749	190,588
TOTAL GROSS POWER	kWe	522,132	480,850
TOTAL AUXILIARY CONSUMPTION	kWe	168,711	100,705
NET POWER OUTPUT	kWe	353,421	380,145
AUXILIARY LOAD SUMMARY			
COAL HANDLING	kWe	593	593
COAL MILLING	kWe	3,008	3,008
COAL SLURRY PUMPS	kWe	601	601
SLAG HANDLING & DEWATERING	kWe	1,504	1,504
AIR SEPARATION UNIT AUXILIARIES	kWe	1,030	1,044
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	kWe	64,878	35,327
OXYGEN COMPRESSOR	kWe	10,551	22,519
NITROGEN COMPRESSOR	kWe	36,649	197
SYNGAS RECYCLE COMPRESSOR	kWe	391	390
TAIL GAS RECYCLE COMPRESSOR	kWe	1,264	-
CO2 PURIFICATION & COMPRESSION	kWe	15,857	19,332
BOILER FEEDWATER & DEMIN PUMPS	kWe	3,457	3,795
VACUUM CONDENSATE PUMP	kWe	213	213
PROCESS CONDENSATE & SWS SYSTEMS	kWe	256	647
HUMIDIFIER & BFW CIRCULATING PUMPS	kWe	20	96
COOLING WATER CIRCULATING PUMPS	kWe	2,920	2,275
COOLING TOWER + AIR COOLER FANS	kWe	4,027	3,129
SCRUBBER PUMPS	kWe	94	94
SELEXOL UNIT	kWe	15,618	-
DESULFURIZER UNIT	kWe	-	1,728
GAS TURBINE AUXILIARIES	kWe	688	626
STEAM TURBINE AUXILIARIES	kWe	88	83
CLAUS & TAIL GAS TREATING AUXILIARIES	kWe	67	-
H2SO4 UNIT	kWe	-	-1,279
MISCELLANEOUS BALANCE OF PLANT	kWe	3,000	3,000
TRANSFORMER LOSSES	kWe	1,934	1,781
NET PLANT EFFICIENCY, HHV	%	28.28	30.42
NET HEAT RATE	KJ/KWH	12731.317	11836.35
	BTU/KWH	12066.96	11218.695
CONDENSER COOLING DUTY NET POWER	10 ⁶ KJ/H	570.703	442.657
	10 ⁶ BTU/H	540.922	419.557
CONSUMABLES			
AS-RECEIVED COAL FEED	KG/H	292294.648	292294.97
	LB/H	644509.699	644510.408
THERMAL INPUT	KWT HHV	1249551.914	1249553.288
RAW WATER USAGE	M ³ /MIN	12.046	13.395
	GPM	3182.659	3539.019
CARBON CAPTURED	%	89.927	90.002

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**Table 4-5
Overall Plant Cost Summary
Subbituminous Coal Cases – Fully Loaded GTs**

	COLD GAS CLEANUP	WARM GAS CLEANUP
UNIT	2007 Installed Cost (\$1000)	2007 Installed Cost (\$1000)
ASU	227,712	235,526
Fuel receiving, preparation & feeding	112,478	114,393
Gasifier, syngas cooler & aux	311,596	316,903
Other Gasification Equipments	68,092	69,252
Syngas scrubber (included in gasification auxiliaries)	0	0
Ash handling systems	39,849	40,528
Shift reactor	15,603	-
Hg Removal	3,147	-
Acid gas removal	207,362	-
Elemental Sulfur Plant	17,939	-
CO2 compression, dehydration & pumping	29,069	-
1st Shift reactor + Combined 2nd Shift & PSA + CO2 compression, dehydration & pumping	-	202,493
Warm gas desulfurization	-	13,440
H2SO4 unit	-	29,363
Blowback gas systems	3,281	3,337
Fuel gas piping	1,690	2,475
Gas cleanup foundations	1,789	3,573
Syngas Humidification	0	-
N2 Humidification	-	2,727
Gas turbine + generator + auxiliaries	132,424	132,424
HRSg, ducting + stack	54,871	55,233
Steam turbine + generator + auxiliaries	54,238	53,111
Surface condenser	30,008	26,415
Feedwater & Misc. BOP Systems	38,194	69,868
Cooling water system	26,858	26,986
Accessory electric plant	90,559	89,849
Instrumentation & controls	27,364	27,364
Improvement to site	19,590	19,924
Buildings & structures	18,471	18,785
Total	1,532,182	1,553,969
Total \$/kW	2,993	2,824

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**Table 4-6
Overall Plant Cost Summary
Lignite Coal Cases – Fully Loaded GTs**

	COLD GAS CLEANUP	WARM GAS CLEANUP
ASU	278,625	290,122
Fuel receiving, preparation & feeding	143,508	153,441
Gasifier, syngas cooler & aux	331,887	354,859
Other Gasification Equipments	72,526	77,546
Syngas scrubber (included in gasification auxiliaries)	0	0
Ash handling systems	57,895	61,903
Shift reactor	17,697	-
Hg Removal	3,252	-
Acid gas removal	224,323	-
Elemental Sulfur Plant	20,613	-
CO2 compression, dehydration & pumping	31,356	-
1st Shift reactor + Combined 2nd Shift & PSA + CO2 compression, dehydration & pumping	-	229,531
Warm gas desulfurization	-	16,229
H2SO4 unit	-	35,459
Blowback gas systems	3,495	3,737
Fuel gas piping	1,685	3,044
Gas cleanup foundations	2,029	4,313
Gas turbine + generator + auxiliaries	137,904	137,904
HRSg, ducting + stack	53,463	57,283
Steam turbine + generator + auxiliaries	58,204	59,596
Surface condenser	32,293	28,902
Feedwater & Misc. BOP Systems	31,893	79,629
Cooling water system	25,585	27,777
Accessory electric plant	95,398	96,287
Instrumentation & controls	27,364	27,364
Improvement to site	20,866	22,310
Buildings & structures	19,674	21,035
Total	1,691,535	1,788,271
Total \$/kW	3,348	2,990

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**Table 4-7
Cost of Electricity
Subbituminous Coal Cases – Fully Loaded GTs
2007 \$**

	COLD GAS CLEANUP	WARM GAS CLEANUP
Net power, MW	511.84	550.35
Capacity factor (CF), %	80	80
Total plant cost (TPC), \$	1,532,182,156	1,553,969,441
6 month labor cost	14,259,309	14,449,993
1 month maintenance materials	2,553,786	2,601,003
1 month non-fuel consumables	376,323	787,430
1 month waste disposal	335,045	415,373
25% of 1 month fuel cost at 100% CF	903,691	925,758
2% of TPC	30,643,643	31,079,389
60 day supply of fuel & consumables at 100% CF	7,872,830	8,857,898
0.5% of TPC (spare parts)	7,660,911	7,769,847
Initial catalyst & chemicals cost, \$	7,295,886	13,388,363
Land	900,000	900,000
Other owners's costs	229,827,323	233,095,416
Financing costs	41,368,918	41,957,175
Total overnight cost (TOC), \$	1,876,179,821	1,910,197,085
Fixed operating cost for initial year of operation (OCF), \$	59,162,262	59,979,374
Annual feed cost at above CF for initial year (OCV1), \$	34,701,738	35,549,111
Other annual variable operating cost at above CF for initial year (OCV2), \$	31,345,478	36,516,530
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year (OCV3), \$	20,696,359	21,171,852
Annual byproduct revenues at above CF for initial year (OCV4), \$	1,491,218	4,666,995
1st year cost of electricity (COE) w/o CO2 TS&M, \$/MWh	99.5	94.6
1st year cost of electricity (COE), \$/MWh	105.3	100.1

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**Table 4-8
Cost of Electricity
Lignite Coal Cases – Fully Loaded GTs
2007 \$**

	COLD GAS CLEANUP	WARM GAS CLEANUP
Net power, MW	505.26	597.99
Capacity factor (CF), %	80	80
Total plant cost (TPC), \$	1,691,535,249	1,788,271,144
6 month labor cost	15,279,234	16,010,475
1 month maintenance materials	2,806,339	2,987,408
1 month non-fuel consumables	360,219	914,213
1 month waste disposal	568,434	718,628
25% of 1 month fuel cost at 100% CF	918,298	1,010,430
2% of TPC	33,830,705	35,765,423
60 day supply of fuel & consumables at 100% CF	7,956,319	9,776,087
0.5% of TPC (spare parts)	8,457,676	8,941,356
Initial catalyst & chemicals cost, \$	8,387,100	16,606,225
Land	900,000	900,000
Other owners's costs	253,730,287	268,240,672
Financing costs	45,671,452	48,283,321
Total overnight cost (TOC), \$	2,070,401,313	2,198,425,380
Fixed operating cost for initial year of operation (OCF), \$	64,389,173	67,786,373
Annual feed cost at above CF for initial year (OCV1), \$	35,262,646	38,800,513
Other annual variable operating cost at above CF for initial year (OCV2), \$	35,855,926	44,354,385
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year (OCV3), \$	23,134,685	25,324,381
Annual byproduct revenues at above CF for initial year (OCV4), \$	1,818,599	6,127,517
1st year cost of electricity (COE) w/o CO2 TS&M, \$/MWh	110.4	99.8
1st year cost of electricity (COE), \$/MWh	117.0	105.8