Final Report

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Integrated Water-Gas-Shift Pre-combustion Carbon Capture Process

Final Report

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Abstract

TDA Research, Inc (TDA) has developed a highly efficient integrated WGS pre-combustion carbon capture technology and demonstrated its techno-economic viability for use in the Integrated Gasification Combined Cycle (IGCC) power plants that process coal. The new system uses a warm gas CO_2 scrubber integrated with a Water-Gas-Shift (WGS) catalyst to capture greater than 90% of the carbon emissions, which does not increase the cost of electricity (COE) as much as conventional carbon capture technologies.

The integrated WGS/CO_2 removal reactor contains both a high temperature physical adsorbent capable of removing CO_2 above the dew point of the synthesis gas and a commercial WGS catalyst to convert CO and H_2O into H_2 and CO_2. The integrated operation of the WGS catalyst and the CO_2 sorbent in a single process step drives the equilibrium-limited WGS reaction towards hydrogen without the need to add large amounts of water to the synthesis gas. When coupled to an IGCC the reduced steam input greatly increases the power cycle efficiency and reduces the cost of carbon capture. Our preliminary system analysis results suggested that maintaining the H_2O:CO molar ratio close to that required by the reaction stoichiometry (i.e., H_2O:CO = 1.0) rather than using an excess of steam (e.g., 2.0 is commonly used as the basis of various DOE analyses) will improve the absolute process efficiency by more than 2% (over a current efficiency of 34%). The process intensification provided by combining the two unit operations in the same reactor will also reduce the capital cost and improve the process economics.

In this project we demonstrated the techno-economic viability of the new process by: 1) demonstrating it in field tests, and 2) carrying out a high-fidelity engineering design and an economic analysis. We fabricated an 8-bed high temperature PSA system to run the full cycle sequence and demonstrated the integrated WGS pre-combustion carbon capture process, including the thermal management subsystems. We completed over 30,000 adsorption desorption cycles, showing stable catalyst and sorbent performance and completed a techno-economic analysis showing the merits of the integrated WGS carbon capture process.

In collaboration UCI, we also completed a high-fidelity process design and economic analysis for the combined WGS based pre-combustion CO_2 capture system integrated with IGCC power plants operating on coal based E-Gas^{TM} and GE gasification systems. This analysis was completed on the basis of the DOE Rev 2a baseline study, operating on Illinois No. 6 bituminous coal integrated with regular state-of-the-art cold gas and TDA's warm gas clean-up based CO_2 capture system (without integration with WGS). We see that the net plant efficiency was the highest for TDA's warm gas capture system when integrated with the last water gas shift stage at 34.7% vs 34.1% for the warm gas capture based system when it is not integrated with the WGS step. The increase in heat rate for the integrated WGS carbon capture system is about 12% over the cold gas cleanup based carbon system (Selexol^{TM}). The cost of carbon capture including TS&M is estimated to be $35.8 per tonne ($25.8 per tonne when excluding the TS&M costs) for integrated WGS based capture system. This is much lower than DOE's target for transformational carbon capture technologies of $30 per tonne excluding TS&M costs.

Table of Contents

List of Tables

List of Figures

Executive Summary

TDA Research, Inc (TDA) has developed a highly efficient integrated WGS pre-combustion carbon capture technology and demonstrated its techno-economic viability for use in Integrated Gasification Combined Cycle (IGCC) power plants that process coal. The new system uses a warm gas CO_2 scrubber integrated with a Water-Gas-Shift (WGS) catalyst to capture greater than 90% of the carbon emissions, with a much lower cost of electricity (COE) increase than conventional carbon capture technologies.

The scrubber consists of a high temperature physical adsorbent capable of removing CO_2 above the dew point of the synthesis gas and a commercial WGS catalyst to convert CO and H_2O into H_2 and CO_2. The integrated operation of the WGS catalyst and the CO_2 sorbent in a single process step drives the equilibrium-limited WGS reaction towards hydrogen, without the need to add large amounts of water to the synthesis gas. When coupled to an IGCC the reduced steam input greatly increases the power cycle efficiency and reduces the cost of carbon capture. Our preliminary system analysis results suggested that maintaining the H_2O:CO molar ratio close to that required by the reaction stoichiometry (i.e., H_2O:CO = 1.0) rather than using an excess of steam (e.g., 2.0 is commonly used as the basis of various DOE analyses) will improve the absolute process efficiency by more than 2% (over a current efficiency of 34%). The process intensification provided by combining the two unit operations in the same reactor also reduces the capital cost and improves the process economics.

In this project we demonstrated the techno-economic viability of the new process by: 1) demonstrating it in field tests, and 2) carrying out a high-fidelity engineering design (Figure 1). In collaboration with Gas Technology Institute (GTI) we designed and fabricated an 8-bed high temperature PSA system to run the full cycle sequence and demonstrated the integrated WGS pre-combustion carbon capture process (including the thermal management subsystems) in field tests at Praxair/Linde's facilities (Tonawanda, NY) using syngas generated by their Oxygen Transport Membrane (OTM) system (Figure 2).

GTI also carried out detailed CFD modeling of the integrated WGS pre-combustion carbon capture process and the thermal management subsystems. Figure 3

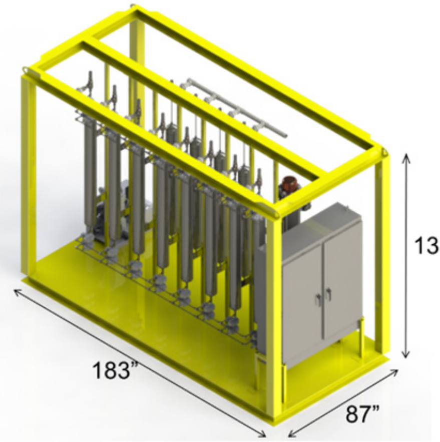


Figure 1.3-D layout of the 10 scfm integrated WGS and CO_2 capture field test unit.

Figure 2. TDA's 10 cfm field unit installed at Praxair's testing location.

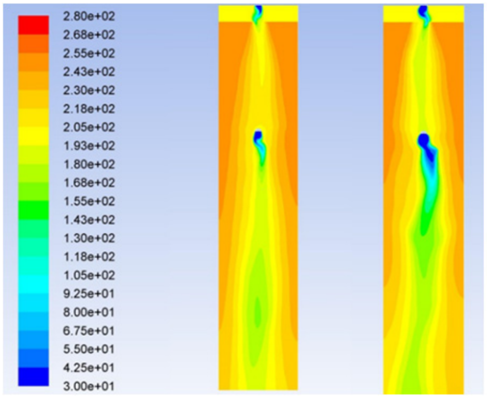


Figure 3. Temperature contours (C) for injection velocity corresponding to 1.0 gal/h total (right) and 0.4 gal/h total (left) split between two axial injectors (Config. C)

shows the Configuration C, which was identified to be one of the more optimal configurations that we developed for the integrated water injection nozzles that are used to remove the heat of WGS reaction from the integrated WGS precombustion reactor. We completed over 30,000 adsorption desorption cycles with the TDA's precombustion carbon capture sorbent integrated with the WGS catalyst in a bench-scale fixed reactor system, showing stable catalyst and sorbent performance. Figure 5 and Figure 4 shows the sorbent and catalyst performance over these long duration multiple cycle tests.

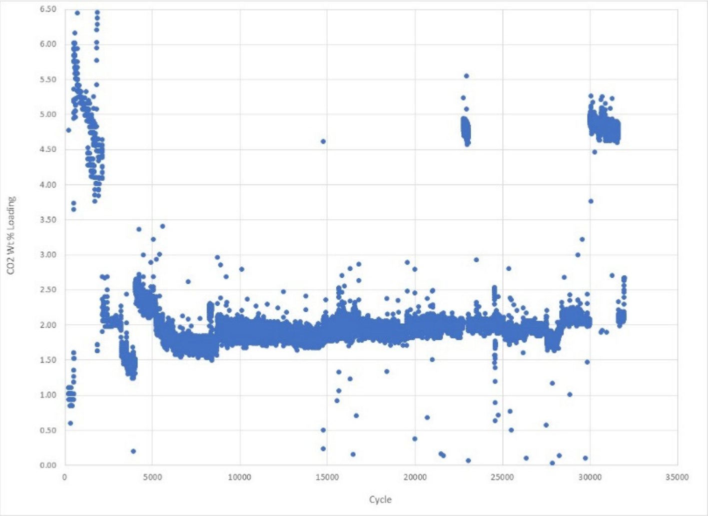


Figure 5. CO_2 loading in sorbent/catalyst cycling data.

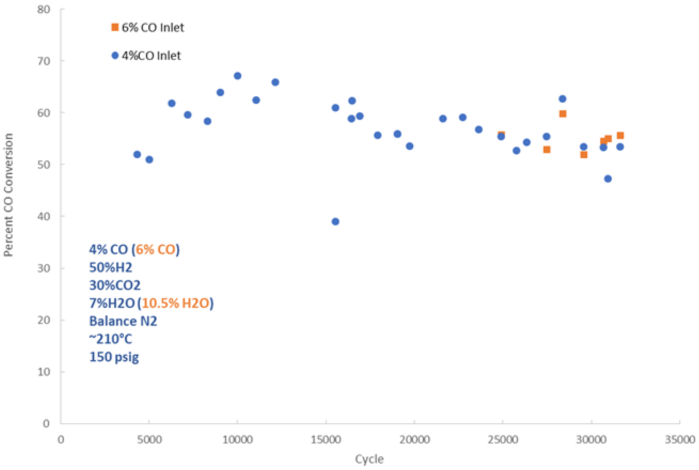


Figure 4. WGS catalyst activity during the long-term durability test of integrated WGS catalyst/CO_2 sorbent bed in bench-scale.

In collaboration with University of California Irvine (UCI) we completed a techno-economic analysis showing the merits of the integrated WGS carbon capture process. UCI completed a high-fidelity process design and economic analysis for the combined WGS based pre-combustion CO_2 capture system integrated to a IGCC power plant operating on either a coal based E-Gas^{TM} or GE gasification system. This analysis was completed on the basis of DOE Rev 2a baseline study. We compared the net plant efficiency and cost of capture numbers for the E-Gas^{TM} gasification system operating on Illinois No. 6 bituminous coal integrated with regular state-of-the-art cold gas and TDA's warm gas clean-up based CO_2 capture system (without integration with WGS). We see that the net plant efficiency was the highest for TDA's warm gas capture system when integrated with the last water gas shift stage at 34.7% vs 34.1% for the warm gas capture based system when it is not integrated with the WGS step. The increase in heat rate for the integrated WGS carbon capture system is about 12% over the cold gas cleanup based carbon system (Selexol^{TM}). For E-Gas^{TM} gasification technology the 1st year CO_2 capture cost without CO_2 transportation storage and monitoring (TS&M) for the Warm Gas Cleanup case is $26/tonne which is significantly lower than that for the Cold Gas Cleanup case at $43/tonne. For General Electric's GEP type gasification technology the 1st year CO_2 capture cost (without CO_2 TS&M) for the Warm Gas Cleanup case is $28/tonne which is significantly lower than that for the Cold Gas Cleanup case at $38/tonne. In the case of coal to liquids processes, the required selling price (RSP) with CO_2 TS&M included for the Fischer Tropsch synthesis of fuels was calculated to be $120/bbl for the manufacture of naphtha and $172/bbl for the diesel in the case of Cold Gas Cleanup, and $115/bbl for the naphtha and $166/bbl for the diesel in the case of Warm Gas Cleanup, a decrease of more than 3% for each of these coproducts.

1. Introduction

TDA Research, Inc (TDA) has developed a highly efficient integrated WGS pre-combustion carbon capture technology and demonstrated its techno-economic viability for use in the Integrated Gasification Combined Cycle (IGCC) power plants that process coal. The new system uses a warm gas CO_2 scrubber integrated with a Water-Gas-Shift (WGS) catalyst to capture greater than 90% of the carbon emissions, while maintaining a low cost of electricity (COE) increase compared to conventional carbon capture technologies.

The scrubber consists of a high temperature physical adsorbent capable of removing CO_2 above the dew point of the synthesis gas and a commercial WGS catalyst to convert CO and H_2O into H_2 and CO_2. The integrated operation of the WGS catalyst and the CO_2 sorbent in a single process step drives the equilibrium-limited WGS reaction towards hydrogen without the need to add large amounts of water to the synthesis gas. When coupled to an IGCC the reduced steam input greatly increases the power cycle efficiency and reduces the cost of carbon capture. Our preliminary system analysis results suggested that maintaining the H_2O:CO molar ratio close to that required by the reaction stoichiometry (i.e., H_2O:CO = 1.0) rather than using an excess of steam (e.g., 2.0 is commonly used as the basis of various DOE analysis) will improve the absolute process efficiency by more than 2% (over a current efficiency of 34%). The process intensification provided by combining the two unit operations in the same reactor will also reduce the capital cost and improve the process economics.

The overall objective of this work was to develop an integrated WGS/pre-combustion carbon capture technology to eliminate CO_2 emissions from Integrated Gasification Combined Cycle (IGCC) power plants. Our specific goal was to demonstrate the techno-economic viability of the new process by: 1) demonstrating it in large-scale slipstream tests, and 2) carrying out a high fidelity engineering design. TDA's process uses an advanced physical adsorbent to selectively remove CO_2 from coal-derived synthesis gas above its dew point. Before we started this project the sorbent's performance had been well-characterized in representative bench-scale experiments and several slipstream field tests using actual coal-derived synthesis gas (DE-FE-0000469; DE-FE-0013105). We had also carried out proof-of-concept evaluations for the integrated WGS/CO_2 removal process and showed that our process can remove carbon with a much higher process efficiency than with the Selexol^{TM} solvent (DE-FE-0007966; DE-FE-0012048).

In this project, we developed, built and tested a slipstream test unit to further demonstrate the merits of the integrated process. We fabricated an 8-bed high temperature PSA system to run the full cycle sequence and demonstrated the integrated WGS pre-combustion carbon capture process. We completed over 30,000 adsorption desorption cycles in a bench-scale fixed reactor system, showing stable performance and completed a techno-economic analysis showing the merits of the integrated WGS carbon capture process.

2. TDA's Integrated WGS and CO_2 Capture Process

TDA's integrated WGS catalyst/high temperature CO_2 scrubber system uses a warm gas CO_2 scrubber based on pressure swing adsorption (PSA) integrated with a Water-Gas-Shift (WGS) catalyst to capture greater than 90% of the carbon emissions with a smaller cost increase in the electricity (COE) caused by competing processes. Figure 6 shows a simplified schematic of our technology integrated with an IGCC plant based on E-Gas^{TM} Gasifier (we used the E-Gas^{TM} system as an example, the proposed technology will work with any gasifier type). In a typical 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.

The particulate-free gas then feeds a water scrubber that operates at 371^{o}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 prevents 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.

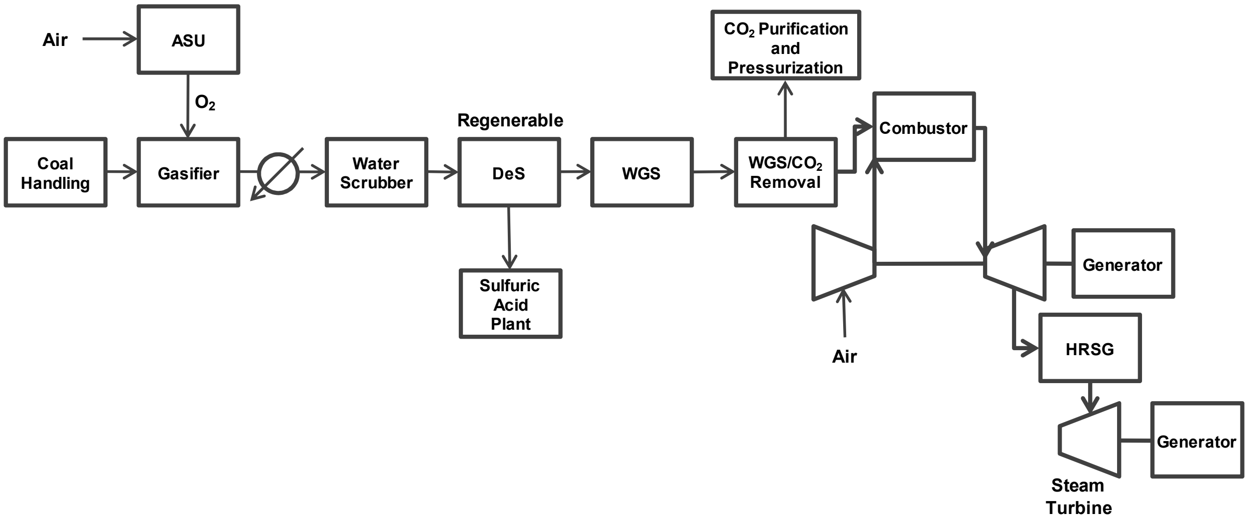


Figure 6. TDA's CO_2 capture system integrated with CoP's E-Gas^{TM} gasifier.

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 Research Triangle Institute (RTI) and Conoco Phillips (CoP) later Chicago Bridge and Iron (CB&I) and now licensed by Sinopec, 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-series shift catalyst. This first stage WGS catalyst bed effectively converts most of the CO and H_2O into H_2 and CO_2. This partially shifted synthesis gas is then sent to our integrated WGS and CO_2 capture bed (that is the basis of our project); this bed uses a combination of low temperature shift catalyst (such as ShiftMax-120 from Sud-Chemie) and TDA's pre-combustion warm gas CO_2 capture sorbent to produce additional hydrogen and capture the CO_2 in a single step.

The integrated WGS/CO_2 capture block consists of a WGS/CO_2 separation system (the high temperature PSA system, which uses a mixed bed of WGS catalyst and TDA's CO_2 sorbent) and a purification/compression system, which further treats the CO_2 stream from the separation unit to produce a pure, pressurized CO_2 product that meets pipeline specifications. TDA's high temperature PSA-based WGS/CO_2 separation system converts the residual CO into CO_2 (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 CO_2 and produces a CO_2-lean synthesis gas (primarily H_2 and H_2O) 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 H_2 recovery in the CO_2 separation unit. A steam purge at lower pressure is used to fully regenerate the sorbent.

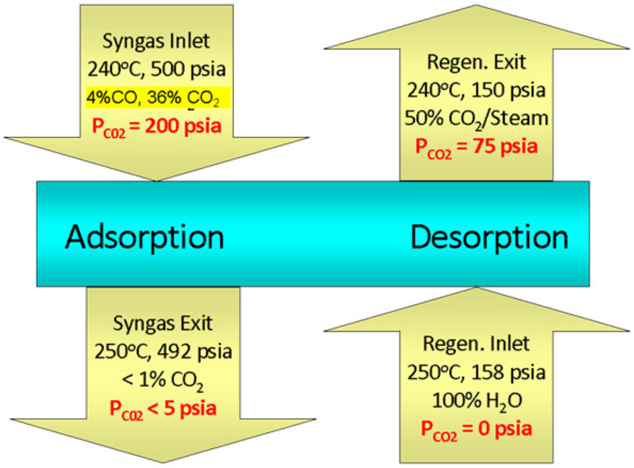


Figure 7. The CO_2 partial pressure swing that drives the TDA's integrated WGS/CO_2 capture.

A CO_2 rich stream, consisting primarily of H_2O and CO_2 (along with some CO and H_2 impurities) is sent for further purification and compression to produce high purity CO_2 at 2,200 psig that can be sent for sequestration. For CO_2 purification a catalytic combustor is used to burn any residual syngas with oxygen. In this approach pure oxygen is used to oxidize any H_2, CO and CH_4 remaining in the concentrated CO_2 stream, converting them into CO_2 and H_2O. After dehydration, CO_2 was pressurized. The catalytic combustion of impurities provided a CO_2 product whose purity is comparable to that achieved by Selexol^{TM}.

3. Project Objectives

In this project TDA Research proposed to work with the Gas Technology Institute (GTI), University of California, Irvine (UCI), Praxair, Indigo Power Systems, the National Carbon Capture Center (NCCC) and Chicago Bridge & Iron (CB&I). We will optimize the reactor design using CFD and kinetic modeling. Based on the new design, we will modify the cycle sequence to optimize CO2 capture and H2 recovery. We will also design a fully-equipped slipstream test unit with 10 SCFM (280 SLPM) raw synthesis gas treatment capacity that will allow us to prove the viability of the new technology. Two field tests will be carried out: at the Power Systems Development Facility (PSDF) at the NCCC, Wilsonville, AL using syngas generated from air blown gasifier and another at pilot gasification facility at Praxair, Tonawanda, NY using oxygen blown gasifier. All results will feed into a techno-economic analysis supported with Aspen Plus^{TM} simulation to calculate the impact of the integrated WGS/CO_2 capture system on plant efficiency and the cost of electricity; all analyses will be consistent with DOE/NETL Cost Estimation Guidelines.

3.1 Work Plan

The project tasks were completed in three budget periods:

Budget Period 1: In Budget Period 1 we will carry out the design of the field test unit and complete sorbent manufacturing based on the existing Manufacturing/Quality Assurance Plans. We will work with GTI to carry out a detailed design of the sorbent reactors, using a multi-component adsorption and CFD simulation models developed in our earlier work. We will design the slipstream test unit, based on the input and with the full approval of NCCC and CB&I. We will also initiate a long-term sorbent life evaluation, running 8,000 cycles. Budget Period 1 is complete.

Budget Period 2: In Budget Period 2, we will complete evaluation of a single integrated reactor and revise our design and commence with the fabrication of the unit. We will continue with the long-term sorbent tests, running 20,000 cycles. Budget Period 2 is complete.

Budget Period 3: In Budget Period 3, we will complete sorbent life tests with 30,000 cycles. We will complete all shakedown, troubleshooting and test trials to ensure flawless operation of the unit before shipping to the demonstration sites. We were initially scheduled to carry out the two test campaigns (one each) at the National Carbon Capture Center (NCCC), Wilsonville, AL and the Wabash River IGCC plant to optimize the system operation and assess its durability under synthesis gas derived from oxygen fired gasifier. However, both the sites have shut down and been decommissioned, so neither could be a host site for this project. TDA secured Praxair (Tonawanda, NY) as the alternate site and will carry out two test campaigns at Praxair site. We will complete the design of the TDA process and also carry out a high-fidelity system analysis i.e., engineering and cost analysis based on vendor quotes for in integrated IGCC power plant and a gasification based CTL plant. Based on the test results we will complete an economic evaluation to accurately estimate the cost of removal of CO_2 using DOE/NETL Cost Estimation Guidelines and complete an Environmental, Health and Safety (EHS) assessment.

4. Accomplishments

The accomplishments in this project were:

Task 1. Project Management and Planning

- We updated the PMP based on comments from DOE project manager and submitted for approval on November 7, 2014 (Milestone 1-1)
- We had a kick-off meeting with DOE on January 9, 2015 over a web conference and presented the project overview (Milestone 1-2)
- We were initially scheduled to carry out the two test campaigns (one each) at the National Carbon Capture Center (NCCC), Wilsonville, AL and the Wabash River IGCC plant to optimize the system operation and assess its durability under synthesis gas derived from oxygen fired gasifier. However, both the sites were shut down and decommissioned during the course of this project. So, TDA held discussions with Praxair and secured access to their Oxygen Transport Membrane (OTM) test facility located in Tonawanda, NY as the alternate site to carry out two test campaigns.
- Due to changes in the field test site and the delays in access to the tests site due to COVID-19, we requested and received no-cost-time-extensions (NCTEs) to complete the project by September 2021
- We held annual review meetings and participated in DOE sponsored topical meetings as required through the course of the project.
- We successfully completed the project and held the Final Review Meeting remotely via webex telecon on August 30, 2021 in which we provided a comprehensive review of the project to the DOE project manager and the gasification team. This completed the Milestone 3-7 on August 30, 2021

Task 2. Detailed Design of the Test Skid

- We carried out the detailed design of the 10 scfm test skid including the 8-bed high temperature PSA beds with integrated WGS catalyst and completed the reactor sizing to provide a basis for CFD modeling
- As part of this task, GTI carried out the CFD model development of the integrated WGS pre-combustion carbon capture process
    - GTI initially completed the calibration of the 2D adsorption CFD model before extending the model to include the integrated WGS and finally extended it to 3-D computational space
    - GTI used the CFD model of the 10 scfm test bed and optimized the heat management scheme
- We completed the detailed design of the 10 scfm test skid, and a preliminary design package was shared with our partners on June 30, 2015 (Milestone 1-3)

Task 3. Design Review and Hazard Analysis

- We completed the initial Design Review and Process Hazard Analysis (PHA) for our 10 cfm test skid on September 30, 2015 (Milestone 1-4)

Task 4. Sorbent Manufacturing

- As part of this task, we worked on improving the volumetric capacity of the sorbents in the scaled up production batches
- We completed the production of sorbents for the field test making about 0.5 m^3 of sorbent on March 31, 2016 (Milestone 1-5)

Task 5. Sorbent Evaluation

- We evaluated the scaled-up sorbent samples in a bench-scale test set up and picked the sample with high CO_2 breakthrough capacity.

Task 6. Reactor Design Optimization

- GTI continued CFD modeling work and optimized the numbers and position of the direct water injection nozzles for heat management of the integrated WGS precombustion carbon capture process, completing Milestone 1-6 on March 31, 2016.

Task 7. Long-term Durability Tests up to 8,000 cycles

- We carried out the multiple cycle life tests in the bench-scale using a modified fixed bed test apparatus that can do counter current flows during adsorption and desorption
- We completed 8,000 adsorption/ desorption cycles with TDA's precombustion CO_2 capture sorbent integrated with WGS catalyst in a bench-scale system on May 14, 2018 (Milestone 1-7)

Task 8. Fabrication of Single Reactor

- We completed the fabrication of the single test reactor that was used to optimize our final design for the reactors used in the field test unit.

Task 9. Evaluation of Single Reactor

- We completed the single reactor tests with the 10 scfm test reactor and explored the use of mechanical steam injectors, which provided us the flexibility to place the injectors inside the PSA beds

Task 10. Reactor Design Revisions

- We revised the reactor test bed configuration to determine the efficacy of the sorbent/catalyst layer layout on CO conversion

Task 11. Fabrication of Single Reactor Revisions

- We completed the single reactor design revisions and fabricated the new reactor configuration

Task 12. Evaluation of Single Reactor Revisions

- We tested the second reactor configuration in the lab using simulated synthesis gas and observed that when using configuration 1, the CO conversion yielded on average 3.5% more CO conversion than configuration 2, completing Milestone 2-1 on June 30, 2016.

Task 13. Long-term Durability Tests up to 20,000 cycles

- We continued the multiple cycle life tests of the integrated WGS precombustion carbon capture bed in the bench-scale fixed bed test apparatus and completed over 20,000 cycles on September 1, 2018 (Milestone 2-3).

Task 14. Critical Design Review

- We completed the critical design review and commenced the fabrication of the 10 scfm field test unit on May 31, 2016 (Milestone 2-2).

Task 15. Fabrication of Field Test Unit

- We completed the fabrication of the 10 scfm field test unit on May 31, 2017 (Milestone 2-4)

Task 16. Shakedown Testing of Gas Processing Skid

- We completed shakedown tests of the gas processing side of the skid on June 30, 2017 (Milestone 2-5)

Task 17. Process Design

- We worked with Indigo Power Systems (IPS) to optimize the concepts and input for integration of the advanced gas turbines into the IGCC to maximize performance
- We updated the AspenPlus® models previously developed by UCI for TDA's integrated WGS pre-combustion capture process integrated to an IGCC power plant
- We completed the sizing and costing for the integrated WGS carbon capture reactor system based on the stream data from the AspenPlus® process model.
- We completed the full-scale process /system design for the CO_2 capture system (Milestone 3-3) on March 30, 2020.

Task 18. Long-term Durability Tests up to 30,000 cycles

- We completed over 30,000 cycles in the multiple cycle life tests of the integrated WGS precombustion carbon capture bed in the bench-scale fixed bed test apparatus on November 13, 2018 (Milestone 3-4).

Task 19. Shakedown Testing of the Slipstream Unit

- We completed shakedown tests of the integrated WGS test skid in July 31, 2017 (Milestone 3-1) and the unit was shipped to Praxair for field tests

Task 20. Field Test at Praxair #1

- We loaded the reactors with catalyst and sorbent and installed the spacers and screens required for the water injection
- We made several trips to Praxair to carry out the initial shakedown and preliminary testing of the 10 SCFM field test unit
- We shared the data from our First field test campaign to our partner GTI so that they could use it in their CFD model validations
  - GTI updated their CFD models to match the exact amounts for the catalyst and sorbent layers
  - Based on the CFD model developed using exact amounts for the catalyst and sorbent layers, GTI ran several steady state simulations, including a baseline (no spray cooling) with and without WGS reactions to verify that the CO_2 sorption process and WGS reactions aspects of the model were functional
- In this first test campaign, we carried out over 60 hours of testing and the tests were completed on June 30, 2018 (Milestone 3-2).
- In the summer of 2019, we went to Praxair and fixed the compressor which malfunctioned in the first test campaign and also verified that the heaters were still operational and flushed out the water injection system and verified that the injection valves and flow meters were functional
- We acquired larger filter housings to replace the smaller tee style filters that clogged so quickly during the last period of operation. This will provide longer periods of sustained operation. The filters were shipped directly to Praxair to be installed immediately before testing will begin.

Task 21. Field Test at Praxair #2

- We traveled to Praxair (now Linde) to repair and modify the apparatus and start the second test campaign
- We carried out tests between September 14 and 27, 2020 using both bottled gases (CO_2 in N_2 mixtures) as well as syngas generated by Linde's OTM panel
- Praxair (now acquired by Linde) was able to get their OTM system tests started shortly after our last travel to Praxair in September, 2020 in this second test campaign we ran for a total of 68 hours on syngas before an issue with condensate collection on Praxair/Linde's OTM panel forced a shutdown.
- Praxair's sump pump broke during this second test campaign with syngas from OTM, and we were able to restart the system remotely. However, we observed increases in pressure drop and issues with syngas flow out of the system.
  - With the help of one of Praxair's engineers, we observed that a large amount of sorbent was escaping the beds making its way downstream and plugging the lines and filters.
- Due to COVID-19 related travel restrictions to New York from Colorado, we could not get the sorbent beds reloaded and the sorbent retention problem fixed. Also, Praxair/Linde had a need coming up for the space we were using for the field tests, so we jointly made the decision to decommission the field unit with Praxair/Linde's help and had it shipped to TDA, completing Milestone 3-5 on December 31, 2020.
- We compiled the data from the Praxair Second Test Campaign to share with GTI for Model validation
- GTI completed CFD Model validation with the data from the Praxair Second Test Campaign

Task 22. System Analysis

- In collaboration with UCI, we completed the Final TEA i.e., system and cost analysis completing the Milestone 3-6 on September 30, 2021
  - For E-Gas^{TM} gasification technology 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $26/tonne which is significantly lower than that for the Cold Gas Cleanup case at $43/tonne
  - For General Electric's GEP type gasification technology 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $28/tonne which is lower than that for the Cold Gas Cleanup case at $38/tonne
  - The required selling price (RSP) with CO_2 TS&M included for Fischer-Tropsch synthesis was calculated to be $120/bbl for the naphtha and $172/bbl for the diesel in the case of Cold Gas Cleanup, and $115/bbl for the naphtha and $166/bbl for the diesel in the case of Warm Gas Cleanup, a decrease of more than 3% for each of these coproducts

5. Results

5.1 Task 1. Project Management and Planning (PMP)

PMP: The project commenced on October 1, 2014 and we updated the PMP based on inputs from the DOE project monitor and submitted it to DOE on November 7, 2014 (Milestone 1-1). We had a kick-off meeting with DOE project manager at NETL on January 9, 2015 (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. We were initially scheduled to carry out the two test campaigns (one each) at the National Carbon Capture Center (NCCC), Wilsonville, AL and the Wabash River IGCC plant to optimize the system operation and assess its durability under synthesis gas derived from oxygen fired gasifier. However, both the sites had shut down and decommissioned during the course of this project. So, TDA held discussions with Praxair and secured access to their Oxygen Transport Membrane (OTM) test facility located in Tonawanda, NY as the alternate site to carry out two test campaigns. Due to changes in the field test site and the delays in access to the tests site due to COVID-19, we requested and received no-cost-time-extensions (NCTEs) to complete the project by September 2021. We held annual review meetings and participated in DOE sponsored topical meetings as required through the course of the project. We held the Final Review Meeting remotely via webex telecon on August 30, 2021 in which we provided a comprehensive review of the project to the DOE project manager and the gasification team, and completed Milestone 3-7. We successfully completed all the project tasks on September 30, 2021. The project Milestone log is summarized in Table 1.

Table 1. Project Milestone Log.

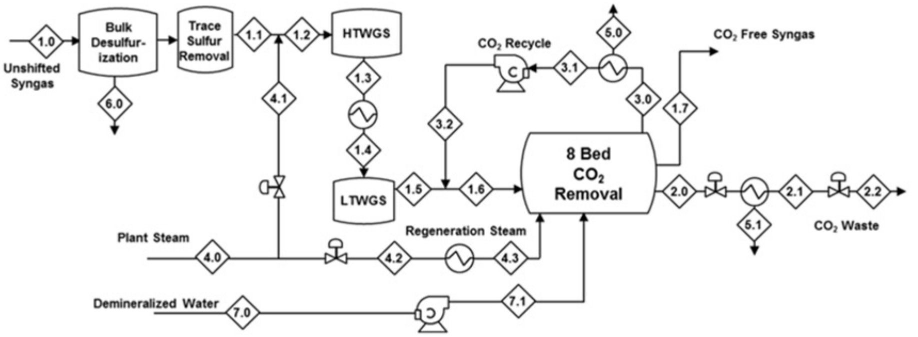
BP	ID	Task No.	Title	Description	Planned Compl-etion	Actual Compl-etion	Verification Method
			Project Start Date		**10/1/14**		
1	1-1	1	Update Project Management Plan (PMP)	Update PMP with inputs from DOE Federal Project Manager	11/3/14	11/7/14	PMP file
1	1-2	1	Kickoff meeting	Kickoff Meeting at NETL	12/1/14	1/9/15	Topical Report - Initial TEA
1	1-3	2	Preliminary Design Package	Provide preliminary design package to field test site operators for feedback	6/30/15	6/30/15	Presentation file
1	1-4	3	Initial Design Review and Hazard Analysis	Complete initial design review and HAZOP	9/30/15	9/30/15	Topical Report - Pilot Plant Design Package
1	1-5	4	Sorbent Manufacturing	Complete the production of the sorbent needed for field tests	3/31/16	3/31/16	Sorbent Manufacturing Plan
1	1-6	6	Reactor design Optimizations	Complete reactor design optimizations	3/31/16	3/31/16	Results update
1	1-7	7	Long-term Durability Target	Complete up to 8,000 cycles at bench-scale	5/14/18	5/14/18	Results update

			I				
1	1-8	1	Annual Review Meeting	Present the BP1 results to DOE/NETL	3/31/16	3/31/16	Preliminary EH&S Risk Assessment Report
2	2-1	12	Single Reactor Evaluations	Complete Evaluation of revised singe reactor	6/30/16	6/30/16	Results update
2	2-2	14	Critical Design Review	Complete the final critical design review	5/31/16	5/31/16	Site Approved SOP for the test skid
2	2-3	13	Long-term Durability Target II	Complete up to 20,000 cycles at bench-scale	10/31/18	9/1/18	Results update
2	2-4	15	Fabrication of Field Unit	Complete the fabrication	5/31/17	5/31/17	Pictures of the Skid
2	2-5	16	Shakedown Testing of Gas Processing Skid	Complete the Shakedown tests using simulated gases	6/30/17	6/30/17	Results update
2	2-6	1	Annual Review Meeting	Present the BP2 results to DOE/NETL	3/20/17	3/20/17	presentation file
3	3-1	19	Shakedown Testing of Integrated Skid	Complete the Shakedown tests using simulated gases	7/31/17	7/31/17	Results update
3	3-2	20	Field Tests at Praxair #1	Complete Field Tests at Praxair #1	6/30/18	6/30/18	Results update
3	3-3	17	Process Design	Complete the full-scale system & process design	3/30/20	3/30/20	Results update
3	3-4	18	Long-term Durability Target III	Complete up to 30,000 cycles at bench-scale	6/28/19	11/13/18	Results update
3	3-5	21	Field Tests at Praxair #2	Complete Field Tests at Praxair #2	8/30/21	12/31/20	Results update
3	3-6	22	System Analysis	Complete System and Cost Analysis	9/30/21	9/30/21	Results update
3	3-7	1	Final Review Meeting	Present the BP3 results to DOE/NETL	12/31/21	8/30/21	Presentation file

5.2 Task 2. Detailed Design of the Test Skid

The primary objective of this project is to carry out a slipstream demonstration with a fully equipped prototype unit. The pilot scale unit is designed to treat at a minimum 300 slpm of synthesis gas flow with a minimum of 15 kg/hr CO_2 capture capability (based on the gas flow at Wabash River IGCC Plant).

Process Flow Diagram (PFD) and Stream Summaries for the Pilot Test Unit



Stream Number		1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	2.0	2.1	2.2	3.0	3.1	3.2	4.0	4.1	4.2	4.3	5.0	5.1	7.0	7.1
Stream Name		Unshif-ted Syngas	S-free Syngas	HTWGS Feed	HTWGS Exit	LTWGS Feed	LTWGS Exit	CO_2 Removal Inlet	CO_2 Free Syngas	CO_2 Waste	Dry CO_2 Waste	LP Dry CO_2 Waste	Cocurr Depress Out	Compre-ssor Inlet	CO_2 Recycle	Plant Steam	WGS Steam	Regen Steam	Cooled Regen Steam	Recyle Condens-ate	CO_2 Condens-ate	In-situ WGS Water	Injected Water
mol %																							
H_2O		20.14%	20.40%	41.06%	23.43%	23.43%	15.68%	14.36%	23.81%	55.74%	2.35%	2.35%	10.35%	1.06%	1.06%	100.00%	100.00%	100.00%	100.00%	99.98%	99.98%	100.00%	100.00%
H_2		24.19%	24.50%	18.14%	35.76%	35.76%	43.52%	42.63%	70.37%	2.55%	5.62%	5.62%	30.57%	33.74%	33.74%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
H_2S		1.27%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
CO		36.49%	36.96%	27.37%	9.75%	9.75%	2.00%	1.82%	0.06%	0.00%	0.00%	0.00%	0.03%	0.03%	0.03%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
CO_2		14.00%	14.18%	10.50%	28.12%	28.12%	35.87%	38.33%	1.23%	41.55%	91.66%	91.66%	57.07%	62.98%	62.98%	0.00%	0.00%	0.00%	0.00%	0.02%	0.02%	0.00%	0.00%
N_2		1.20%	1.22%	0.90%	0.90%	0.90%	0.90%	0.88%	1.40%	0.05%	0.11%	0.11%	0.62%	0.68%	0.68%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
HCN		0.01%	0.01%	0.01%	0.01%	0.01%	0.01%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Other (C1, Ar, NH_3)		2.70%	2.73%	2.02%	2.02%	2.02%	2.02%	1.98%	3.13%	0.11%	0.25%	0.25%	1.36%	1.51%	1.51%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Vapor Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
Molecular Weight	g/mol	21.9	21.7	20.7	20.7	20.7	20.7	21.5	7.4	28.3	40.9	40.9	28.0	29.1	29.1	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0
Temperature	°C	193	193	193	330.0	190.0	220.0	207	200	200	37	37	200	37	176	315	288	280	200	37	37	20	20
	°F	379	379	379	626	374	428	405	392	392	99	99	392	99	349	599	550	536	392	99	99	68	68
Total Flow	gmol/h	758.0	748.4	1010.6	1010.6	1010.6	1010.6	1111.4	620.4	901.8	408.7	408.7	111.2	100.8	10.4	767.6	262.3	505.3	505.3	10.4	493.1	16.8	16.8
	SCFM	10.0	9.9	13.3	13.3	13.3	13.3	14.7	8.2	11.9	5.4	5.4	1.5	1.5	0.1	10.1	3.5	6.7	6.7	0.0	0.0	0.0	0.0
	lb/h	36.5	35.8	46.2	46.2	46.2	46.2	52.7	10.1	56.4	36.8	36.8	6.9	6.5	0.7	30.4	10.4	20.0	20.0	0.4	19.5	0.7	0.7
Pressure	psig	357	354	352	345.2	345.2	337.9	338	331	68	25	7	73	73	338	325	352	68	68	73	25	68	1450
C_p	J/mol C	32.5	32.9	33.5	36.4	34.7	35.7	35.8	31.0	38.4	37.0	37.0	38.1	34.5	37.9	36.3	36.0	35.9	35.1	75.4	75.4	75.4	75.4
Dew Point/T_{sat}	°C	146.3	146.3	167.0	148.0	148.0	136.6	133.9	148.6	120.8	37.0	26.3	84.4	37.0	65.4	212.4	180.0	118.9	118.9	-	-	-	-
Specific Gravity		12.0	11.8	11.2	8.5	11.1	10.2	10.9	3.7	3.4	3.6	1.9	3.6	5.6	15.7	7.1	8.1	1.8	2.1	1.0	1.0	1.0	1.0

Figure 8. Stream Summaries and PFD.

The test unit consists of two parts: (1) the Gas Conditioning Unit and (2) the combined WGS and high temperature pressure swing adsorption (PSA) based CO_2 Separation Unit. The primary function of the synthesis gas conditioning unit was to adjust the concentration and purity of the synthesis gas. The unit was originally designed for operation with both synthesis gas derived from air blown and oxygen blown gasifiers. We have used National Carbon Capture Center (NCCC) located in the Power Systems Demonstration Facility at Wilsonville, AL and the Wabash River IGCC power plant as model sites for the two cases, respectively. Because it is setup as a test site, the NCCC had all the capabilities of shifting the synthesis gas (converting the CO into CO_2 via water-gas-shift reaction), the Wabash River IGCC plant has no such capabilities. We have initially carried out the stream summary calculations for the NCCC test site using a sulfur free synthesis gas (Figure 8). The sulfur free synthesis gas (Stream 1.0) enters the Gas Conditioning Unit (GCU) where the gas is mixed with steam from the test site and enters the low temperature water gas shift sub-system, where the CO-rich synthesis gas is partially converted to CO_2 and H_2 before entering the PSA Unit. This partially shifted synthesis gas enters the PSA Unit and the gas flows through one of the PSA beds containing both sorbent and Low temperature WGS catalyst where the rest of the CO is converted to CO_2 and all the CO_2 in the synthesis gas is captured while the other beds are either depressurizing or being regenerated using steam purge.

5.2.1 CFD Modeling

In pursuit of a fully calibrated combined Water-Gas Shift (WGS)/CO_2 adsorption computational fluid dynamics (CFD) model, GTI worked with TDA to identify potential accuracy gaps in assumptions built into both the adsorption and WGS models. GTI investigated numerous available options and, in reviewing results, selected the simplest option that allowed for flexibility and required the fewest assumptions. By matching trends to the experimental data, absolute comparisons with temperature fields and breakthrough are used for calibration.

Model Modifications to Setup

As mentioned previously concerning the modeling of the combined sorbent/WGS-catalyst mixture, the WGS reaction parameters from the *Review of the Water Gas Shift Reaction Kinetics*[1] document for the Sud-Chemie EX-2248 were very successful at describing the performance of the ShiftMax 230 WGS catalyst used in the experimental datasets. For reference, these inputs are shown in Table 2.

Table 2.Main properties used in the 2-D 8-Bed Model.

Properties	**External Porosity**	**Bulk Density (kg/m^3)**	**Bulk Heat Capacity (J/kg*K)**	**Bulk Thermal Conductivity (W/m*K)**	**Physical/Chemical Reaction Details**
Sorbent	0.3	354	700	0.5	**Absorption:** $k_b = 0.1788 \exp\left(-\frac{504.2}{T}\right);$ **Desorption:** $k_b = 0.0405 \exp\left(-\frac{514.6}{T}\right);$
WGS-Catalyst	0.3	1860	546	29.99	**WGS-Forwards*:** $k = 2.96e5 \exp\left(-\frac{5701.2}{T}\right);$ $r = kP_{CO}P_{H2O}$
Sorbent/WGS-Catalyst Mix	0.3	440	946	12.17	N/A

* For Süd-Chemie EX-2248, from Choi and Stenger (2003)

The following assumptions were used, to calibrate the model results to the dataset provided by TDA in a file dated April 2013; obtained as part of a prior DOE funded contract #DE-FE0007966 in a field test campaign at National Carbon Capture Center (NCCC) in April 2013:

- Inlet gas at 0.66 g/s is 7.52% CO, 9.14% CO_2, 7.17% H_2, 8.32% H_2O, and balance N_2. This mixture enters the reactor at 170°C.
- Operating pressure of the 4” ID, 32” long cylindrical vessel is 200 psig (caps of vessel are neglected). Internal wall temperatures are at 200°C.
- The upper 6.35” and lower 6.35” of the vessel are sorbent only, starting the simulation at 200°C and 170°C respectively. The center portion of the vessel, 18” tall, is initially 210°C. As the bulk of the mixed sorbent/catalyst bed is sorbent, 71% by volume and 61% by mass,

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[1] Smith, B. et al. “Review of the Water Gas Shift Reaction Kinetics”, Int’l Journal of Chemical Reactor Engineering, Vol. 8, 2010.

the viscous resistance constants for the sorbent alone from the prior modeling are still in use.
- As the sorption and, more importantly, catalyzed water gas shift (WGS) reaction occur primarily on solid surfaces, GTI initially investigated the use of surface chemical reactions, with a known site surface to volume ratio, as an alternative to a simplified gas-phase volumetric reaction. This value was estimated using the estimated site density for *Shiftmax 230* of 93.09 m^2, the known catalyst mass, and the vessel combined sorbent/catalyst volume of 3.914 L. The results proved inaccurate in comparison to volumetric reaction modeling, due to the assumed adsorption/desorption rate kinetics. For sake of simplicity, GTI continued with volumetric gas phase reactions, as is the case with the adsorption mechanism.

This basic methodology yields the following results:

- **TemperatureField** – The temperature field within the bed is governed by (a) the large effect of the heat of adsorption, (b) the thermal diffusion within the bed and convection of the moving gases entering at 170°C, and (c) the influence of the constant temperature wall surface. In Figure 9, the general trends of each temperature probe from the April 2013 dataset are captured, but the magnitude of change is not correct.

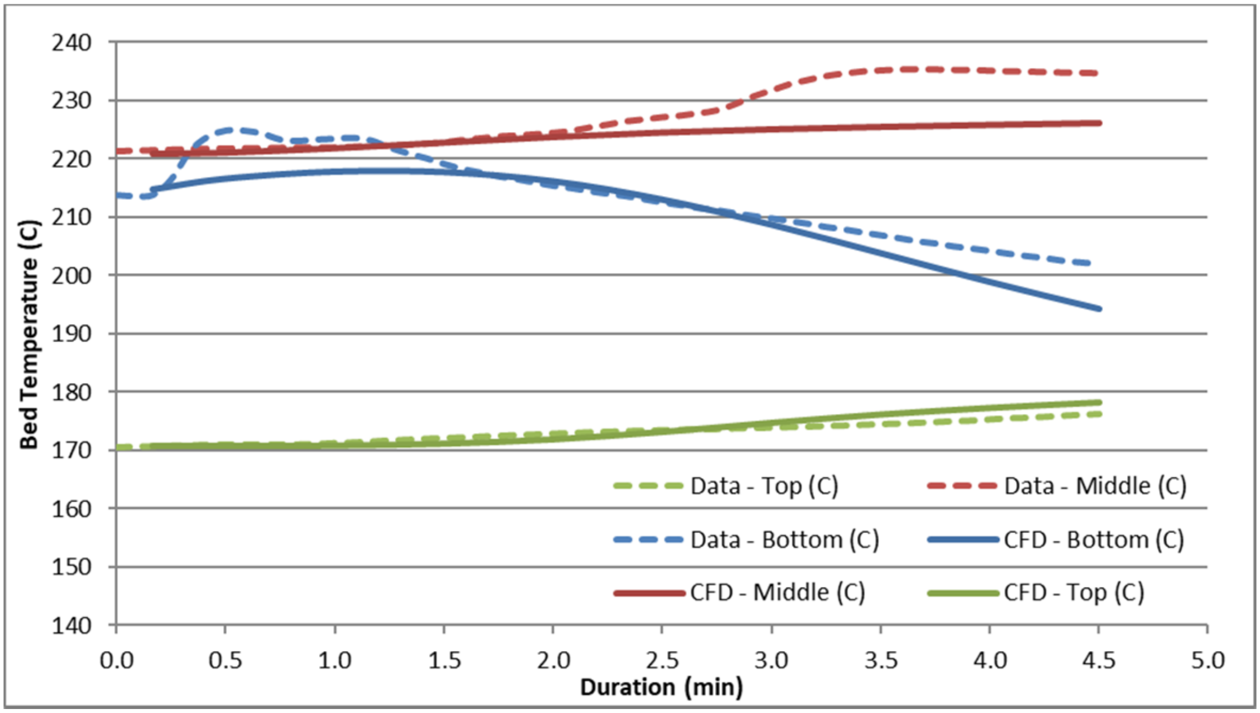

Figure 9.Temperature comparison between baseline CFD model and dataset provided by TDA dated April 2013 (previously obtained as part of DE-FE0007966).

It can be seen in Figure 9 that the middle temperature in the CFD model does not match that of the experimental dataset (the deviation approximately 5°C towards the end of the adsorption cycle), though the bottom and top sections show very good agreement. The 5°C under-heating in the middle is a function of the WGS reaction and under-predicting adsorption. Viewing the bed temperature distribution at the end of the 4.5 minute adsorption cycle (Figure 10) shows a high temperature at the transition from the bottom, sorbent-only, portion, to the middle, sorbent/catalyst, section. Concerning the distribution of adsorbed

CO_2, also shown in Figure 10 in the middle diagram, this transition shows a relative minimum of adsorbed CO_2 as the partial pressure of CO_2 in this region is low prior to generation of CO_2 from the WGS reaction. Thus, whereas the bulk of heating within the vessel is known to be from the heat of CO_2 adsorption, this spike in temperature is in fact due to a compression of the WGS reaction zone, which can be seen in the right-hand diagram of Figure 10. The middle zone shows significant reaction rate decay with elevation, which is due to the artificially high WGS reaction rate, to be discussed in a later section.

- **Breakthrough –** Whereas the temperature field shows good agreement, though slight underestimation of the heat of adsorption, this is also reflected in the breakthrough. Figure 11 shows scaled output of CO and CO_2 mole fractions (wet) that indicate (a) full breakthrough of CO_2 occurs shortly after 3 minutes have elapsed, (b) that the CO_2 “wave” is diffusing although the WGS reaction is clearly active as (yCO_2_out)/(yCO_2_in) exceeds 1.0, and (c) that CO consumption is not optimized, with unconverted carbon exiting the vessel. Note that concerning (c), that the WGS is showing near complete conversion, which would be represented by a value of (yCO_2_out)/(yCO_2_in) = 1.822 (without adsorption).

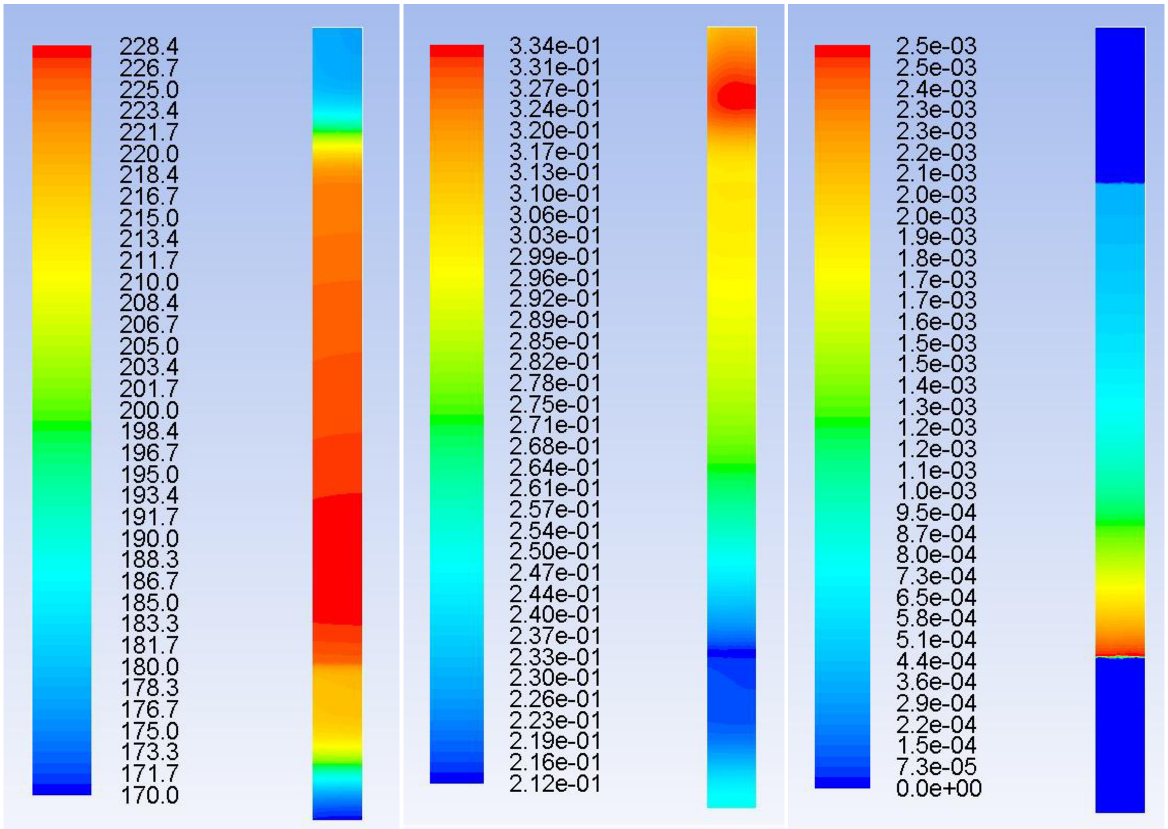

Figure 10.Baseline model bed temperature on left (°C), adsorbed CO_2 in middle (mol/kg), and WGS reaction rate on right (kmol/m^3-s) at 4.5 minutes.

From this baseline model, it is apparent that the assumptions outlined previously lead to:

- Inadequate adsorption rate of CO_2, leading to earlier breakthrough of CO_2 and lower than expected release of the heat of adsorption (lower peak temperatures). The adsorption mechanism must be adjusted.
- Maldistribution of the WGS reaction, simultaneously yielding slight excess unconverted CO in the exhaust and a drop by an order of magnitude of WGS reaction rate along the

elevation of the combined sorbent/catalyst portion. As the WGS forward reaction is thermodynamically favored at lower temperatures, increasing the bed temperatures through greater CO_2 adsorption will further affect this issue, thus slight adjustments to the WGS reaction rate may be necessary.

Modification – Water-Gas Shift Rate Parameters

The Arrhenius rate parameters outlined in Table 2 yield a rate constant k_{WGS} which is determined for a specific case as outlined in the reference. This reference indicates that the test case is slightly different than what it is used to approximate the *Shiftmax* catalysts used in the calibration testing. The reference data from Choi and Stenger are for: (a) a lower CO/H_2O ratio of 1:2 compared to close to 1:1 in the TDA data and (b) finer grain catalyst pellets at 200-250 μm versus the 0.13" long pellets in the TDA data (3,300 μm). These are competing effects, as the former will result in underprediction while the latter will result in overprediction. The sensitivity of an adjustment to the pre-exponential factor *A*, which acts as volumetric efficiency adjustment relative to the reference data, will be explored as well. With competing dynamics, it is not certain how to approach this calibration *a priori*.

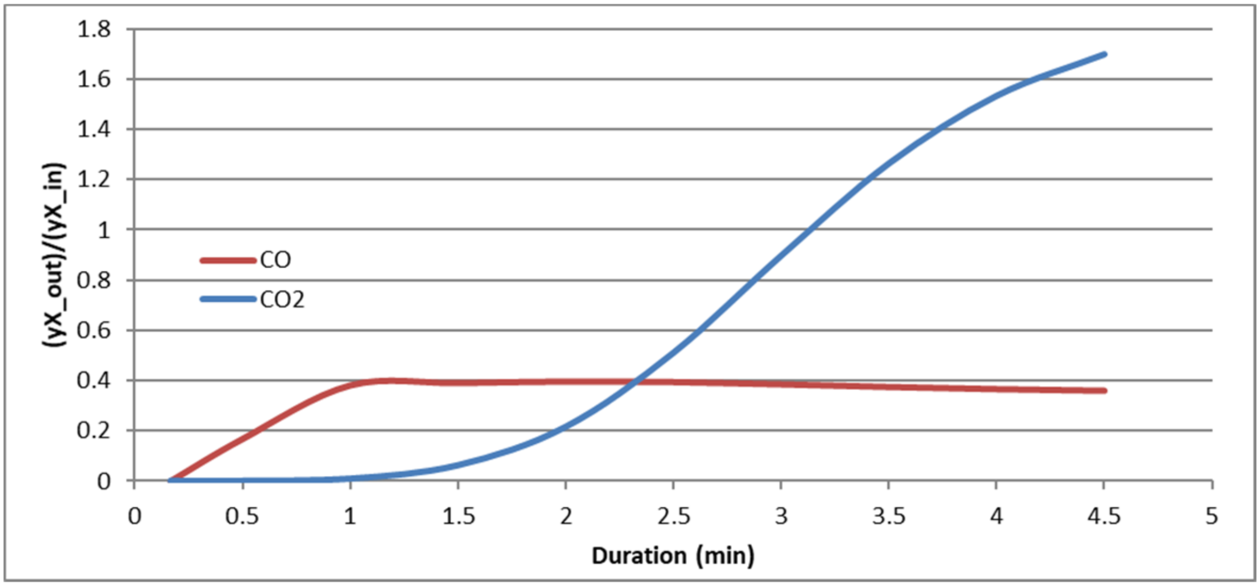

Figure 11.Baseline model breakthrough as y_{CO} and y_{CO2} at vessel outlet.

Modification - CO_2 Adsorption Rate

Using the established Langmuir-Freundlich model ("L-F" model), the maximum adsorbed CO_2 capacity of the vessel with a CO_2 partial pressure of 35.8 psia[2] and a temperature of 200°C is 0.395 mol CO_2/kg sorbent. As the bed has 2.12 kg and the combined inlet molar flow of CO/CO_2 is 0.246 mol/min, breakthrough would occur with this simple 1-D analysis after 3.4 minutes. Incidentally, this is rather close to the results shown in Figure 11, noting that the results are biased low by incomplete CO conversion and high by modeling a non-zero thickness CO_2 "wave". Per input from TDA[3], laboratory data from the 4-bed system for a CO_2 partial pressure of 38 psia at 200°C (close to these conditions), the total adsorbed CO_2 was 0.59 mol/kg sorbent. Using the formulae outlined by TDA, shown in Figure 12, the parameter q_s was modified. This term, the adsorption capacity of the system (number of sites per mass of sorbent) is modified via the constant k_1. Through simple fitting of the aforementioned TDA

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[2] Assumes 100% CO conversion.

[3] Email correspondence dated March 16th, 2015.

laboratory data, this constant is increased by 42.5%, which in effect recalibrates this value more accurately to these lower pressure data, whereas the constants in the model outlined in Figure 12 were fit to data up to partial pressures of 600 psia.

$$q = \frac{q_s BP^n}{1 + BP^n}$$

q (mol CO_2/kg); P (psia)

$$q_s = k_1 e^{k_2/T}; B = k_3 e^{k_4/T}; n = k_5 e^{k_6/T}$$

Figure 12.L-F Model.

In addition to this recalibration of the term q_s, the impact the rate constant k_b is also examined. This constant, outlined in Figure 13, is based on lower pressure data, where the data published by TDA indicate that a CO_2 partial pressure of 12 psia results in a rate constant of 0.065 s^{-1}, using the curve fit in Figure 13, this corresponds to a bed temperature of 225°C. By contrast, for the CFD calibration case of a partial pressure of up to 35 psia, the use of this curve fit may result in underestimation of the adsorption rate. In addition to adjusting the factor k_1, GTI also experimented with using higher, fixed rate constants for k_b, from 0.06 to 0.20 s^{-1}. Note that per this model, wherein this rate constant is a function of bed temperature, for the range of bed temperatures expected between 170°C and 220°C, this yields a +/- 5% variation in rate constant, thus the error introduced by removing this temperature dependency is not expected to be large.

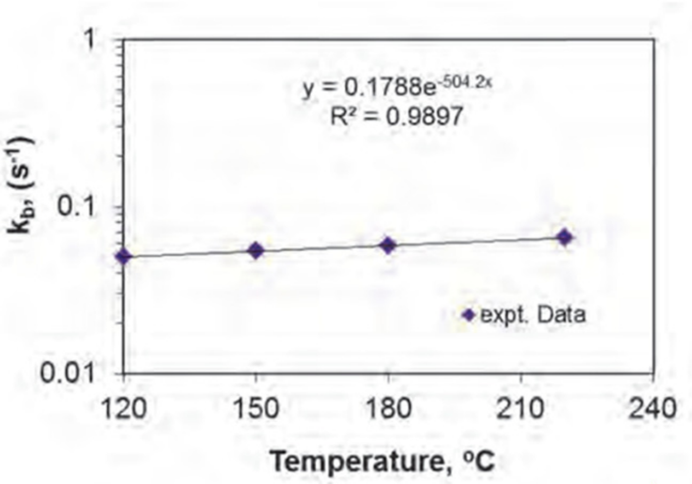

Figure 13.Derivation of adsorption rate constant k_b[4].

Improvement of Baseline Model

In Table 3, the parameters varied, their ranges, and the number of variants simulated are shown, summarizing inputs for a 25 case parametric run. Concerning the issue of CO_2 adsorption kinetics, the issue is well characterized and thus the analysis is limited; however, the WGS rate adjustment required several cases to understand impacts. Also sensitivity is taken to the fact that these issues are not independent, greater CO_2 adsorption drives the WGS reaction forward and greater conversion of CO yields more CO_2 to adsorb.

Table 3.Variation on modeling assumptions to adsorption and WGS reaction rate kinetics.

Calibration Concern	Variable Input	Lower Range	Upper Range	Variants
Insufficient CO_2	Adjustment to k_1	1.0	1.425	2

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[4] Alptekin, G. “A Low Cost, High Capacity Regenerable Sorbent for Pre-combustion CO_2 Capture” prepared by TDA Research for the US DOE, Contract DE-FE0000469 (2012).

Adsorption	Constant Value for k_b	0.06	0.20	4
WGS Rate Adjustment	Adjustment to A	0.3	1.5	5

First, examining the impact of the WGS rate adjustment, retaining the original assumptions outlined in Table 2 otherwise, the direct impact of these changes to the WGS rate constant values on CO conversion is clear per Figure 14, which is to be expected. With a lower value for A, the additional CO_2 decreases with a proportional increase of CO, however this impact is not linear, due to the aforementioned interactions. Thus, adjusted in isolation, a lower value of A increases time to breakthrough, but by an inaccurate method of decreasing the conversion rate.

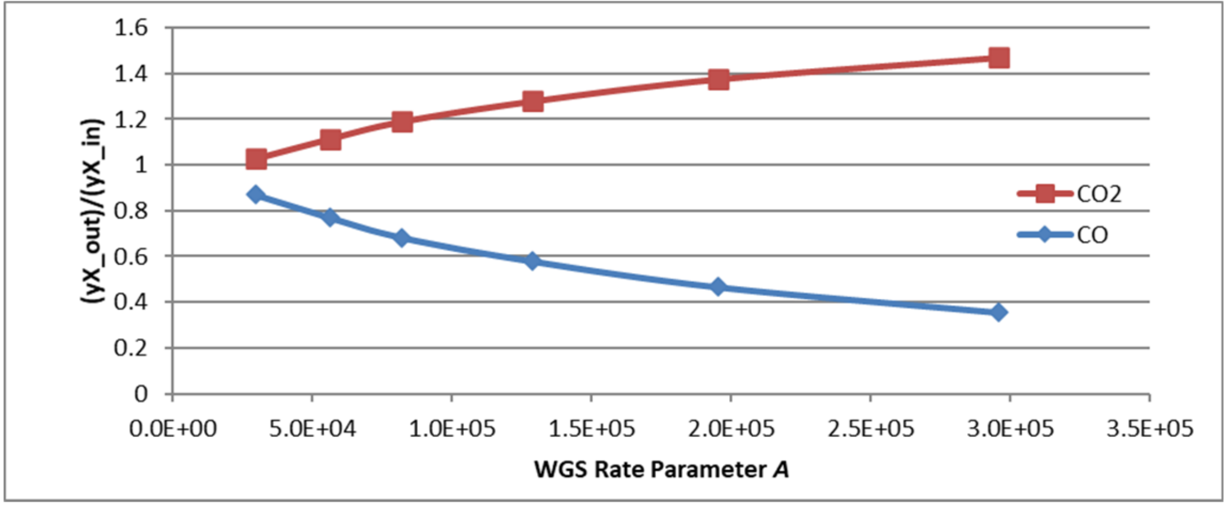

Figure 14. Impact of WGS parameter *a* on outlet CO/CO_2 mole fractions at 4.5 minutes for baseline assumptions.

Adjusting the value k_1, increasing by 42.5% as indicated previously, and varying a constant value for the adsorption rate constant k_b, the impact appears to be muted shown in Figure 15. Note that the impact of adjusting k_1, shown for the $A = 2.96 \times 10^5$ case, is significant in comparison to the final CO_2 value shown in Figure 11, a decrease in 35% and near alignment with predicted breakthrough at 4.5 minutes duration. Thus, while the parameter k_b has a less significant impact, the higher value of 0.20 clearly yields results more in line with test data.

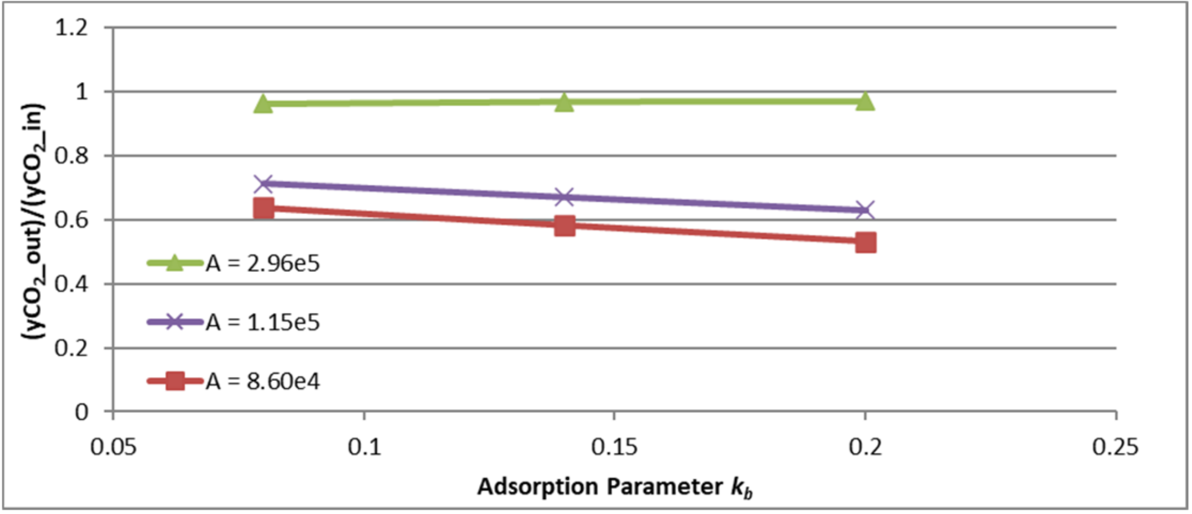

Figure 15.Impact of parameter k_b on outlet CO_2mole fractions at 4.5 minutes by pre-exponential constant *A*.

In a final case, the impact of viscous resistance parameters are studied, where the baseline model assumed that the pressure loss of the sorbent-only bed (from prior analysis) was sufficient for this bed with portions of mixed sorbent/catalyst, where these viscous parameters correspond to pressure drops of 1.2 psi and 11.6 psi respectively. This impact is shown below in Figure 16, highlighting the increase in outlet CO_2 with a greater pressure drop. For a greater pressure loss, it is feasible that downstream of the vessel inlet, the lower local partial pressure of CO_2 yields reduced local adsorption rates, hence higher outlet CO_2 in the gas phase.

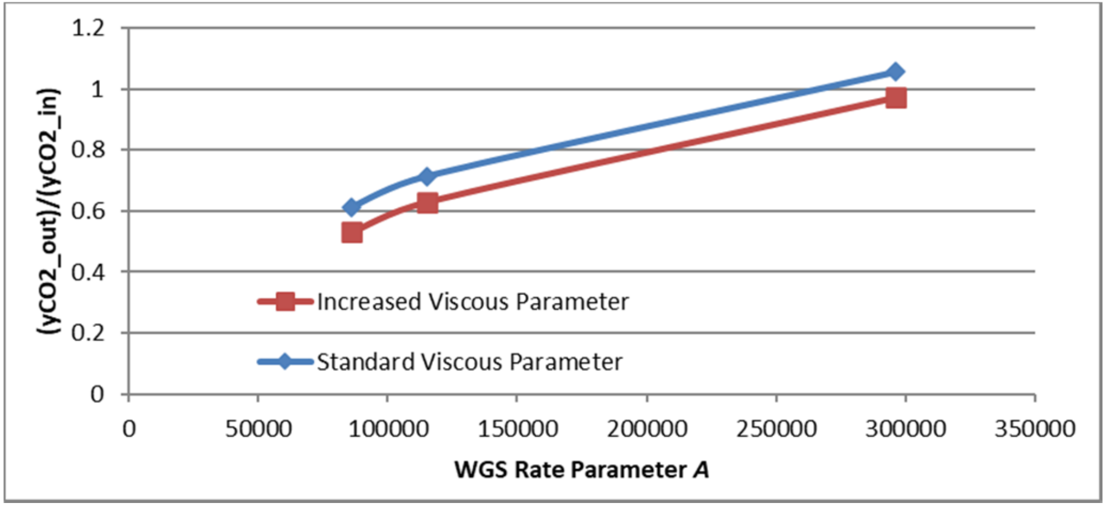

Figure 16. Impact of increasing baseline viscous parameter by order of magnitude, with k_b = 0.20, and an increased k_1 at 4.5 minutes.

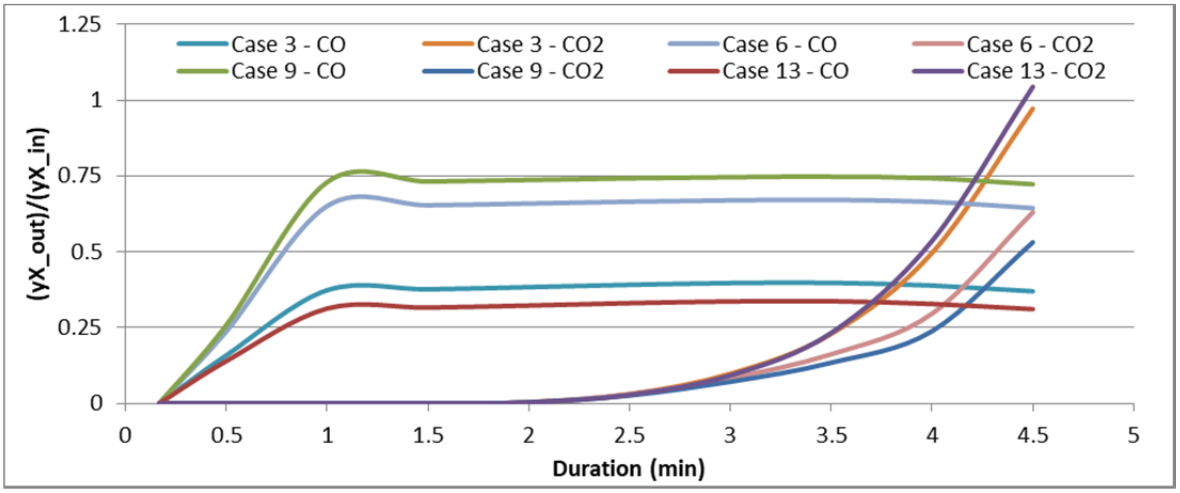

Figure 17. Modified model breakthrough as y_{CO} and y_{CO2} at vessel outlet

Examining the breakthrough data for those cases with k_1 increased by 42.5%, k_b = 0.20, and A varied from baseline values (2.96e5) as "Case 3", to reduced values shown in Figure 15 of 1.15e5 (Case 6) and 8.6e4 (Case 9), these data are summarized in Figure 17. Additionally, the impact of increasing the WGS shift reaction parameter A by 25% is captured in Case 13. For all cases, the impact of the adsorption parameter adjustments is clear, with breakthrough duration[5] increased for all cases. The impact of slowing the WGS reaction, shown moving from Cases 3 to 6 to 9, is inaccurate, as it delays breakthrough by limiting the CO conversion. Including

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[5] Breakthrough defined as when outlet scaled CO_2 mole fraction is equal to 1.0.

assessment of other cases not shown, Case 3 provides the best agreement with breakthrough while requiring fewer ad hoc adjustments, only the increase in k_1 and value of k_b at a constant 0.20 s^{-1}.

Examining this “Case 3”, shows promising results as the CO outlet is unaffected compared to baseline predictions (Figure 11), but breakthrough is nearly exact at the target of 4.5 minutes. The comparison to the bed temperature field is shown in Figure 18 for this case, which shows slightly better agreement than in Figure 11. As such, this Case 3 was used primarily going forward.

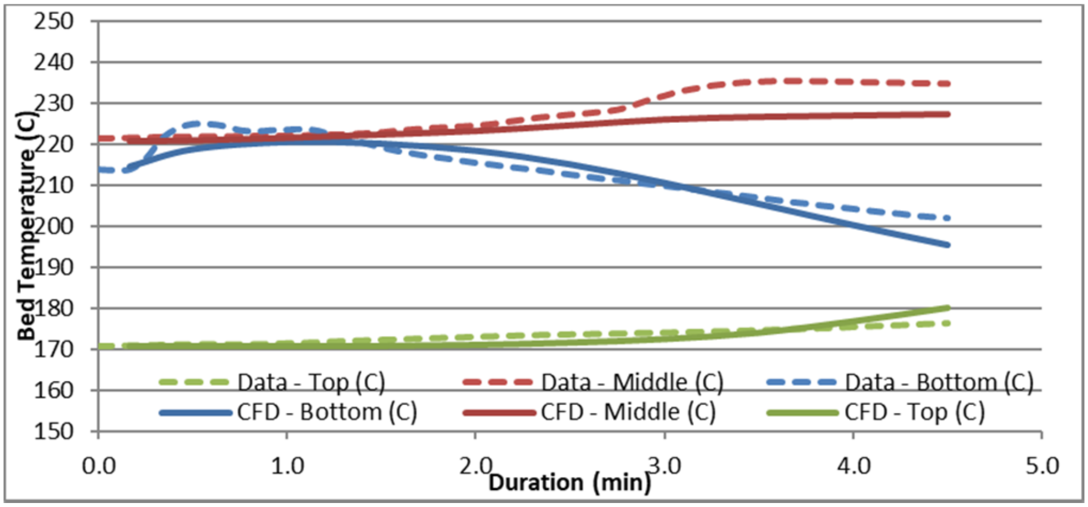


Figure 18. Temperature comparison between modified “Case 3” CFD Model and April 2013 Dataset

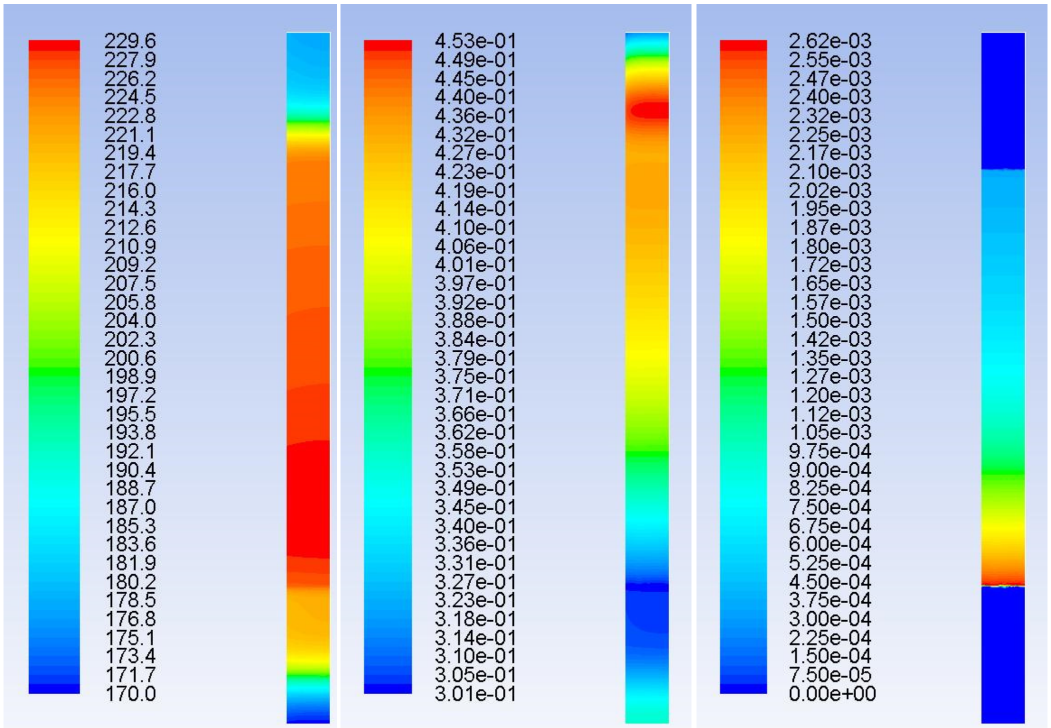
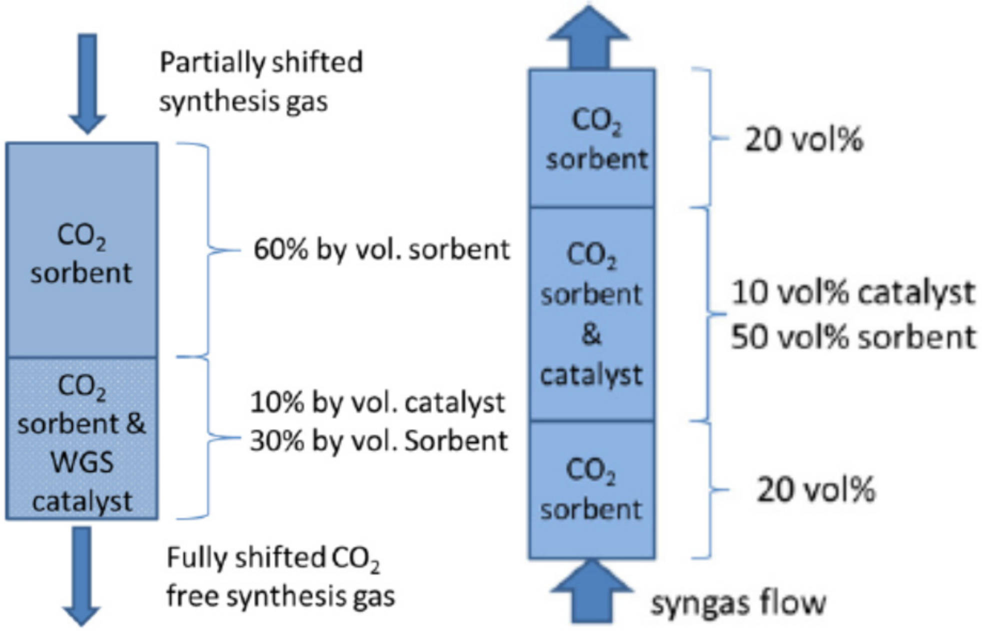


Figure 19. Case 3 model bed temperature on Left (°C), adsorbed CO_2 in middle (mol/kg), and WGS reaction rate on right (kmol/m^3-s) at 4.5 minutes.



Split Bed Tri-Layer Bed

Figure 20.Bed configurations for the integrated WGS/CO_2 sorbent reactor.

Thermal Management Schemes for Integrated WGS catalyst/CO_2 Capture System

The Integrated WGS catalyst/CO_2 Capture System for evaluation of thermal management schemes identified in this task will therefore integrate the 2nd low temperature WGS subsystem with the CO_2 removal unit. Two possible configurations of the integrated WGS/CO_2 sorbent reactor with a catalyst/sorbent ratio of 10% by volume are shown in Figure 20. In-order to limit the temperature rise to ≤40°C (for optimum sorbent performance) in the integrated WGS/CO_2 sorbent reactor the combined heat released by the exothermic WGS and CO_2 adsorption reactions needs to be removed using an effective method. To accomplish this, two heat removal schemes, a cooling jacket surrounding the reactor and tubes or coils or slotted/multi-orifice tubes submerged in the reactor with water as cooling medium were selected for initial evaluation. Examples of cooling jackets and submerged tubes are shown in Figure 21.

Table 5 is a summary of all the heat management systems that were explored during this project. Next we describe the process as well as advantages and disadvantages of each system.

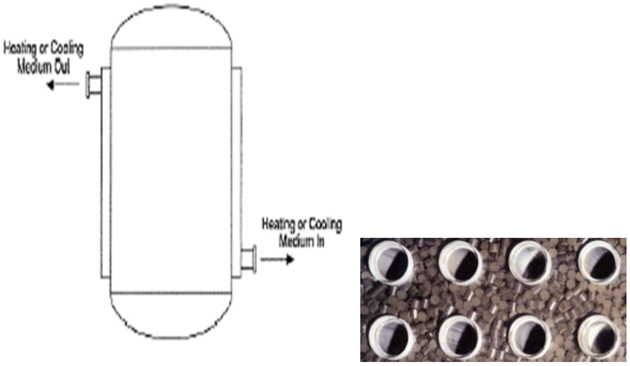


Figure 21.Reactor with cooling jacket (left) and cut-through of tube bundle submerged in bed & surrounded by sorbent/catalyst particles (right).

Table 4. Heat Management Schemes for the Integrated WGS/CO_2 Separation Sorbent Reactor

Description	Advantages	Potential Issues
External Processes		
Cooling jacket (full or dimpled) surrounding the reactor and using water or other heat transfer fluids, e.g. synthetic organic or silicone.	• Provides good coverage of reactor outer surface area and simple to construct. • Dimpled jacket allows construction from light gauge metals while maintaining strength and providing adequate heat transfer area.	• May require high fluid flow rates for adequate heat transfer. • For exothermic reactions, a jacketed vessel has the disadvantage that the area/volume ratio decreases with increasing scale.
Half-pipe or limpet coil jacket welded on the outside of the vessel to provide more contact area versus a cooling coil wrapped around the vessel.	• Improvement over the jacket to obtain good heat transfer of the cooling fluid around the reactor periphery.	• Limited amount of surface coverage.
Internal Processes		
Tube coils or straight or finned tubes or slotted or perforated tubes submerged in the bed wherein water as coolant flows through the tubes.	• Large heat transfer area can be provided, especially with finned tubes. • Results in good heat transfer.	• Impose additional pressure drop to syngas flow, and affect bed temperature distribution.
Evaporative cooling by direct injection of water through a porous sintered stainless steel membrane tube such as the Pall Accusep Inorganic Membrane.	• Provides steam for WGS and effectively utilizes water heat capacity. • Localized temperature control in the WGS /sorbent portion of bed. • Low resistance to coolant flow, high surface area, and good thermal conductivity for heat transfer.	• Synchronization of water injection rate with heat removal rate could be a challenge.
Shell-and-tube type heat exchanger, wherein the catalyst and sorbent are packed inside tubes and water in the shell side as coolant.	• Effective heat transfer due to intimate coolant contact.	• Complex valving and manifolding to attain uniform gas flow through tubes and perform PSA.
Cool feed syngas from the upstream WGS stage to below dew point so that the gas has suspended droplets of water that evaporate on contact with the catalyst/sorbent bed material to provide cooling.	• Liquid water flashing/evaporation provides better heat removal than vapor injection.	• Control of water content in the syngas stream may be a challenge. • Risk of catalyst or sorbent damage due to thermal shock.

Description	**Advantages**	**Potential Issues**
Heat pipe or thermosyphon submerged in bed. A sealed system containing a liquid, which when vaporized transfers heat under isothermal conditions. The heat pipe has three major operating zones: evaporator, adiabatic section and condenser. In the case of simple pipe design, liquid returns from the condenser via a wick structure. The wick is designed to provide a capillary pumping action. In the thermosyphon there is no wick structure and liquid is returned to the evaporator by gravity.	• Can achieve high heat transfer in the system. • WGS catalyst can be coated on the heat pipe surface in contact with sorbent.	• External scheme required to cool heat transfer fluid for reuse. • Same issues as with submerged tube coils.

5.2.2 Reactor Design

We also estimated the reactor size for the 10 CFM Integrated WGS/CO_2 capture system based on the expected composition of partially shifted synthesis gas for Wabash River Field test conditions. We used the estimate from our Aspen modeling of the full-scale system with bituminous coal and E-Gas^{TM}gasifier for the 1st WGS stage. Table 5 shows the composition of the raw synthesis gas entering our field test unit and the partially shifted synthesis gas composition entering WGS/CO_2 capture unit. Table 6 shows the reactor size estimated for the 10 CFM Integrated WGS/CO_2 capture system. The reactors will use a 6” Sch 40 pipe and end caps made of stainless steel.

Table 5.Partially Shifted Synthesis Gas Composition entering WGS/CO_2 capture unit.

Stream Name		**Raw Syngas entering gas conditioning skid**	**WGS/CO_2 removal feed**
H_2O	mol. %	19.9%	10.6%
H_2	mol. %	23.9%	44.4%
H_2S	mol. %	1.3%	0.0%
CO	mol. %	36.1%	4.7%
CO_2	mol. %	13.8%	36.1%
N_2	mol. %	2.4%	2.0%
Other	mol. %	2.7%	2.21%
Temperature	°C	193.8	200
Pressure	PSIG	356	350
Total flow	gmol/hr	621.6	759.6
	SCFM	8.2	10.0

Table 6.10CFM unit reactor size estimate.

Partially shifted Syngas	10.0	scfm
CO_2 flow	13.3	kg/hr
CO_2 Captured	95%	
	12.6	kg/hr
CO_2 Capacity	4.0%	wt.
Adsorption step time	1.5	min
Sorbent needed	7.9	kg
	22.9	L
Sorbent density	0.345	kg/L
Catalyst needed	2.2	kg
	1.2	L
Catalyst density	1.833	kg/L
Total Bed volume	24.1	L
Bed Internal Diameter	6.07	"
Bed Length	50.9	"
L/D	8.4	

5.3 Task 3. Design Review and Hazard Analysis

TDA performed an initial design review and Process Hazard Analysis (PHA) on the field test unit design. The objectives of the PHA were to identify hazards that could lead to consequences of interest and implement design or operational methods to mitigate these risks. The consequences of interest that was explored were injury to personnel, endangerment to the public and the environment, significant equipment damage and system downtime. The system was broken down into separate nodes while each piece of equipment in that node underwent a deviation analysis. For each deviation, potential causes along with their potential consequences were hypothesized. From there, each deviation was assigned a level of risk based on the criteria stated above. If the risk was deemed significant, a list of current safeguards (pressure relief valve, interlocks and alarms, etc.) was created to ensure that there was a low probability that a high-level consequence would occur. If the current design's safeguards were deemed inadequate, a design change was recommended and implemented.

Along with safeguards, a detailed operations manual was created in order to operate the apparatus safely. The manual details system start-up, operation and executing the experimental testing plans and properly shutting down the system.

Lastly a Failure Mode and Effects Analysis (FMEA) was performed on the system. This report assigned rankings to various failures according to their severity and likelihood. For example, a severe event (potential life-threatening injuries/death and/or >2 million dollars in damage) with a high probability is given a high ranking where lower-level events (no potential injuries and/or little to no damage) is given a low ranking. Every moderate to high level ranking was analyzed for potential measures that can lower their rankings to low or negligible. These measures can include both design and operational implementations. The risks are then reevaluated and assigned another ranking which takes into account these measures

Figure 22. TDA's 2" Bonnot laboratory screw extruder

For the integrated WGS/CO_2 sorbent system, a total of 219 events were identified. 155 of these are considered negligible or low risk. 15 events are considered moderate risk and 49 events are considered high risk. After taking into account the safety measures of the design and operation of the system and revaluating the risk ranking, all 219 events were considered negligible to low risk.

5.4 Task 4. Sorbent Manufacturing

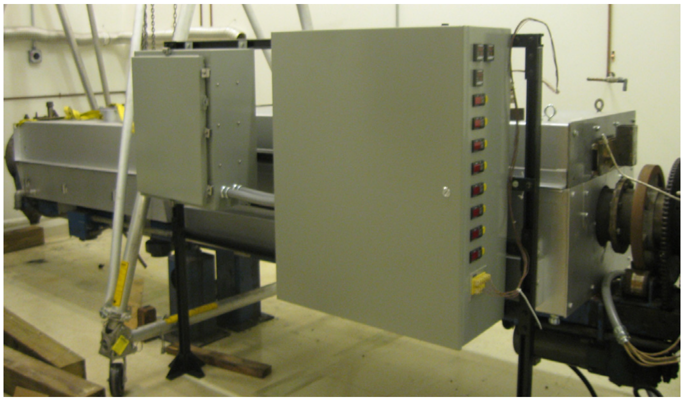


Figure 23. TDA's 7" rotary kiln.

As part of this task, we worked on improving the volumetric capacity of the sorbents in the scaled-up production batches. We used high throughput production equipment including a Littleford plow mixer and a Bonnot 2" laboratory stainless steel screw extruder to make 1/16" pellets (Figure 22). These pellets were then carbonized and activated using a Bartlett and Snow continuous rotary kiln (Figure 23). The rotary kiln is electrically heated and has a 7” Inconel tube that can be heated up to 1100°C. The carbon precursor is fed into the kiln using a single screw feeder. It has a computer control system using Labview software. It has all the safety features needed to operate safely and an afterburner to process the off gases in an environmentally sound manner.

Finally, following the preparation procedures for the best scaled-up batch, we completed the production of sorbents for the field test about 0.5 m^3 on March 31, 2016 (Milestone 1-5)

5.5 Task 5. Sorbent Evaluation

The sorbent prepared in our large rotary were evaluated in a bench-scale test set up. Figure 24 shows the CO_2 breakthrough results from two of the formulations being evaluated, each had a different active precursor and the surface area (AMS-185 was 1,000+ m^2/g while AMS-235 was between 400-500 m^2/g).

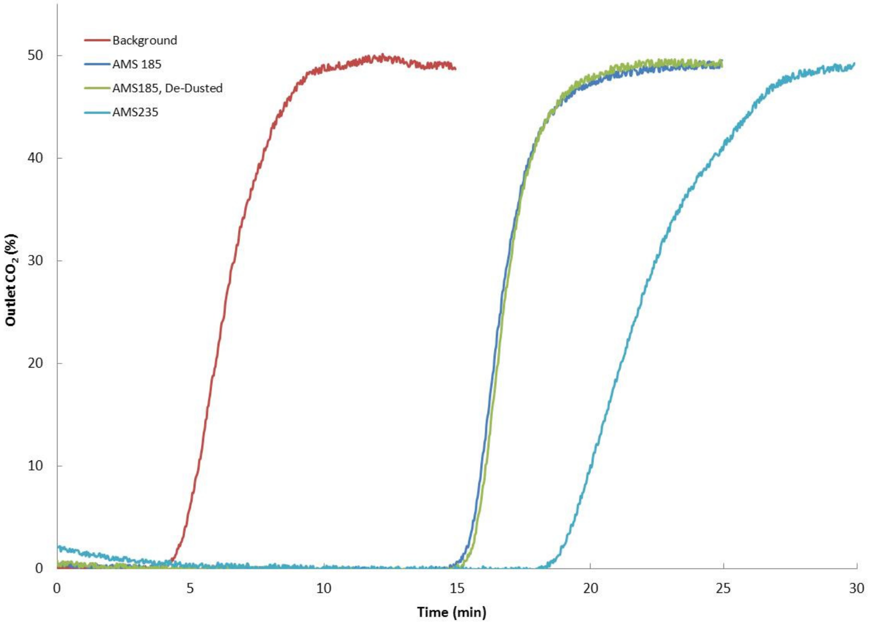


Figure 24. CO_2 breakthrough: 200°C, 300 psig, 50% CO_2, 50%N_2 Inlet, 100% N_2 Regen, 250h^{-1}

5.6 Task 6. Reactor Design Optimization

In order to optimize the reactor design, we modeled a 10 scfm reactor (6” ID vessel), with three configurations – distributed catalyst (configuration A), a single catalyst layer (configuration B), and a dual catalyst layer (configuration C) with all cases having the same quantity of catalyst (5% of total vessel volume). Figure 25 shows the three configurations. The total heat release from the shift reaction for the 10 scfm test skid is approximately 350 W and the goal for direct water injection is to absorb this heat with minimal hot/cold spots. The heat absorption takes place in three phases, sensible heat (18%), phase change (40%), and superheat (42%), assuming peak bed temperature is 250°C for a baseline water flow rate of ~0.6 lb/hr. We also evaluated both axial and radial injection. In axial injection case, water is sprayed co-current with syngas flow and in the radial injection case water is sprayed from side of vessel, which resulted in partial quenching of the shift reaction with

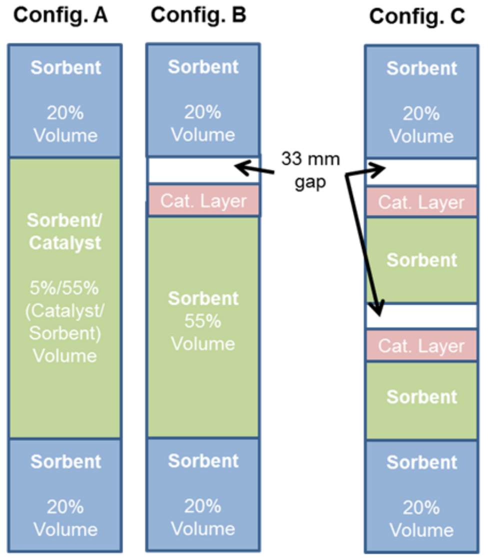


Figure 25.Different configurations explored in CFD modeling for catalyst distribution in the combined WGS/PSA beds.

liquid water streaming along one side (Figure 26).

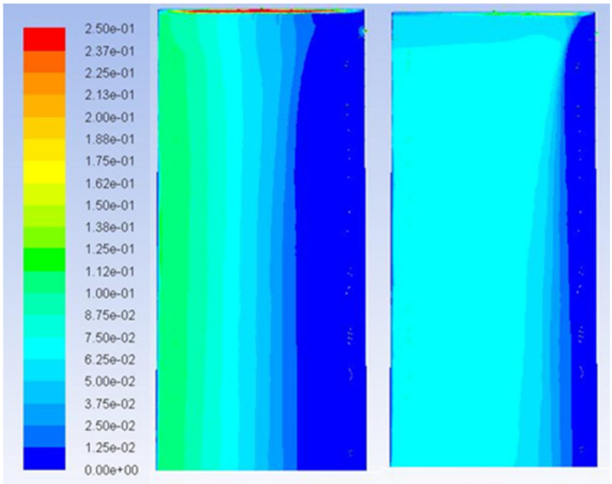


Figure 26. Temperature contours (C) for water injection flowrate corresponding to 2 gal/h (left) and 0.4 gal/h (right), resulting in overcooling along the injection side wall.

Axial Injection – Distributed Catalyst (Config. A)

Axial injection of water results in a cooling pattern similar to that of embedded tubes (3), with good temperature distribution 1-2 dia. downstream of catalyst section, but hot spots remain near spray and overcooling occurs after 3 dia. downstream. For higher water injection rates, an instability develops that may represent a physical phenomenon, whereby zones along spray path have the shift reaction quenched, spray condenses, shift reaction recovers, re-vaporizes the spray and so forth. This results in mildly oscillatory temperature field. Figure 27 shows the horizontal temperature profile at midpoint of the catalyst sorbent mixed layer (y=38.5” from bottom) for various water injection flow rates (gal/hr).

Axial Injection – Catalyst-Only Layer (Config. B)

Similar to the distributed catalyst configuration (A), we observed that hot spots remain near spray and overcooling occurs after 3 dia. downstream. For higher water injection rates oscillations were seen. The impact on the temperature field is more dynamic, as spray precools the syngas prior to exposure to catalyst layer. The resulting temperature field is similar to embedded tubes (3 tubes). This shows that we can eliminate three internal cooling tubes by having a single water injector. Figure 28 shows the temperature contours for single catalyst layer and axial injection (config. B)

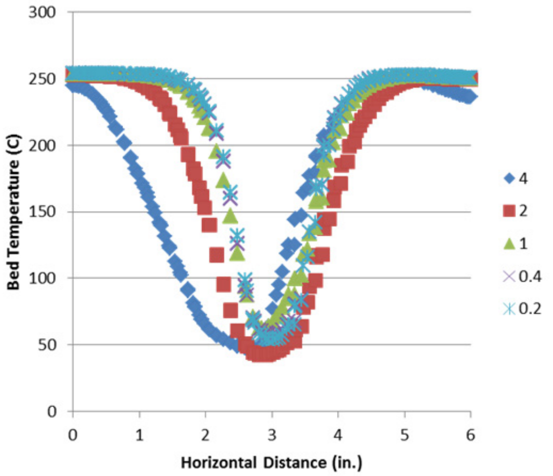


Figure 27. Horizontal temperature profile at midpoint of the catalyst sorbent mixed layer (Config. A) y=38.5” from bottom for various water injection flow rates (gal/hr).

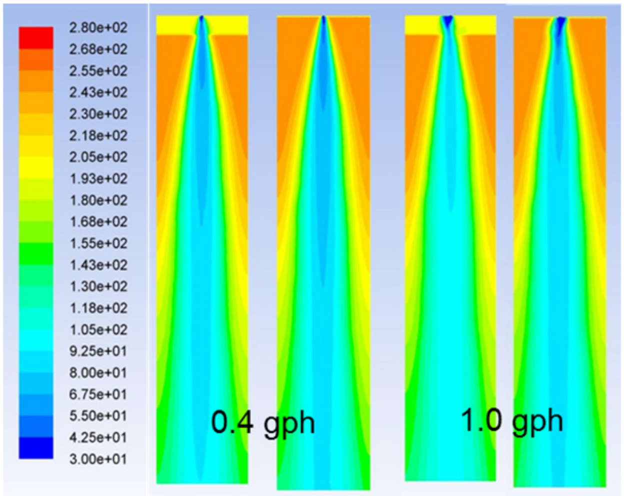


Figure 28. Temperature contours (C) for injection velocity corresponding to 1.0 and 0.4 gal/h for axial injection with (right) and without (left) catalyst-only layer (Config. B) .

Two Axial Injection – Two Catalyst-Only Layers (Config. C)

This configuration provided the best (optimal) heat management, providing even cooling and temperature control. The two injectors provided the operational flexibility to control the temperature individually in the two catalyst layer zones. This configuration also minimized the downstream overcooling in comparison to other injector options. Figure 29 shows the temperature contours for two axial injections with two catalyst layers (Config. C). Figure 30 shows the horizontal temperature profile at midpoint of the top catalyst only layer (y=38.5" from bottom) for various water injection flow rates (gal/hr).

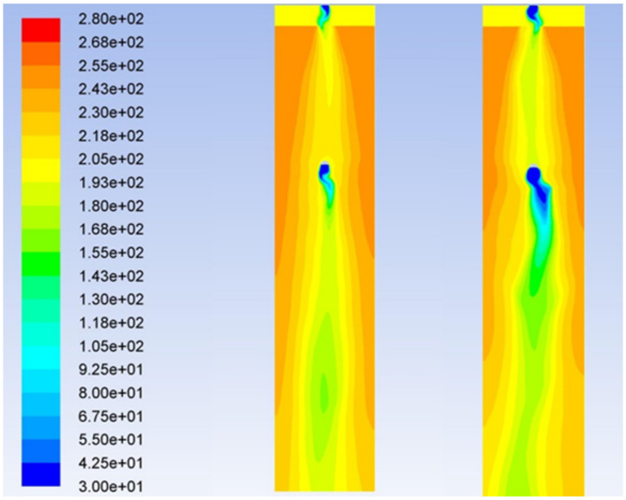


Figure 29. Temperature contours (C) for injection velocity corresponding to 1.0 gal/h total (right) and 0.4 gal/h total (left) , split between two axial injectors (Config. C) .

We performed CFD modeling work pertaining to the optimization of the number and position of the direct water injection for heat management in the integrated WGS/CO_2 sorbent 6-inch reactor. Although axial spray-cooling proved effective at limiting bed temperatures to 200°C and below while avoiding over-cooling, the radial distribution of a single nozzle per elevation proved to be sub-optimal. The case of low (left) and high (right) water flow rates for two spray nozzles, each above a 33 mm (1.3") gap followed by a catalyst-only layer and a sorbent-only layer is shown in Figure 29. The temperature contours indicate that the peripheral sections of the bed are not cooled substantially until downstream of the second spray nozzle. This suggests that the radial distribution of nozzle spray is insufficient. Additionally, the even spacing of two elevations of nozzles may be insufficient as well. From prior test data and baseline CFD simulation validation, it is known that the bulk of heat liberated from the water-gas shift (WGS) reaction occurs in the top of the vessel. Figure 31 shows for the validated baseline simulation of the 6" vessel (no integrated cooling), the proportion of heat generated by the WGS reaction as a function of distance. Using this data, 50% of the total WGS heat of reaction is liberated within the first third of the catalyst/sorbent bed. Thus, it is critical to focus cooling on this upper section, while adequately cooling the lower sections without quenching the WGS reaction. It was therefore decided to continue the modeling effort by grouping it into two segments: (1) optimization of nozzle quantity/placement for a single elevation (top) and (2) optimization of multi-nozzle/multi-elevation.

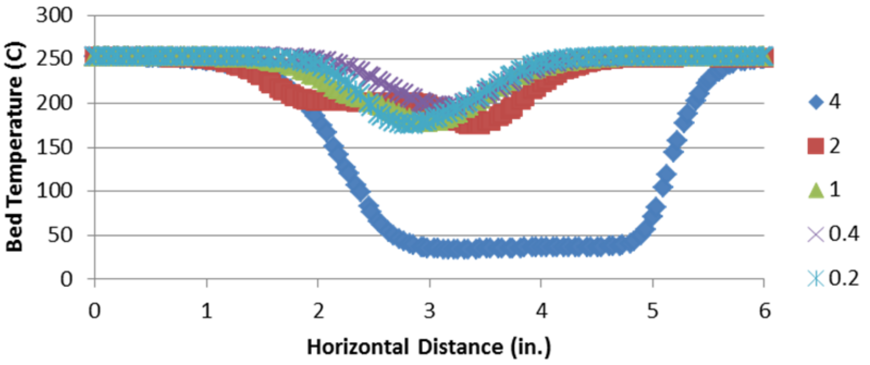


Figure 30. Horizontal temperature profile at midpoint of the top catalyst only layer (Config. C) for various water injection flow rates (gal/hr).

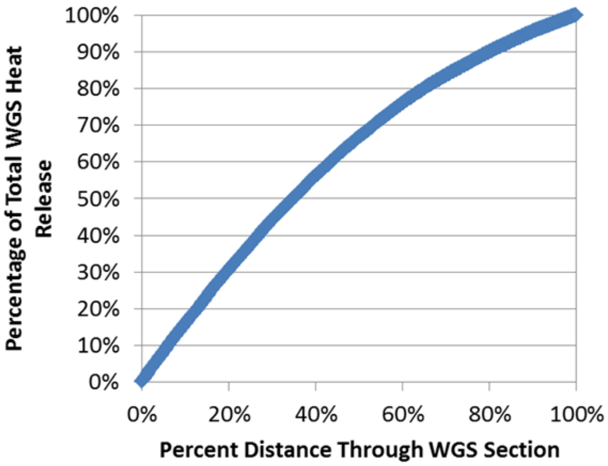


Figure 31. Proportion of WGS reaction heat generated over length of combined catalyst/sorbent.

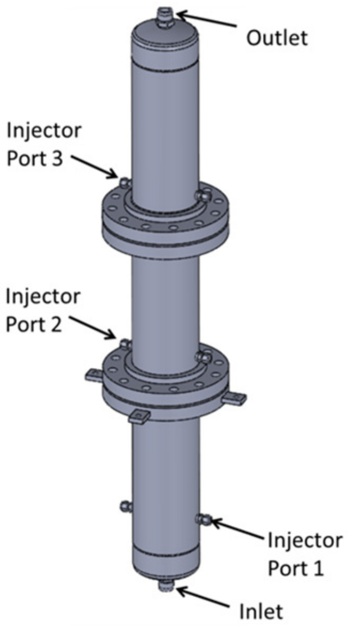


Figure 32. 3-D Reactor Layout.

5.7 Task 8. Fabrication of Single Reactor

The single test reactor (Figure 32) was made from 6-inch schedule 40 304 SS steel pipe with 300# 304 SS flanges. The inlet and outlet are 1” VCR glands. The reactor was built in three sections in order to gain access to the internals of reactor once it’s been built. This was done to allow testing of different bed configurations in order to optimize each sorbent/catalyst section. The reactor was wrapped in heating tapes and insulated. Removable internal baffles were made to separate each section and allow a gap for the water to be sprayed. These baffles consist of two circular perforated plates joined by threaded rod. Around the edge is a Teflon gasket, which prevents sorbent from moving between the baffle and the wall of the reactor.

Figure 33 shows the fully fabricated single reactor. The single test reactor was hydrostatically tested to 2.5 times the operating pressure and was held for 2 hours to determine if there were any leaks.

Figure 33. Single test reactor.

We tested various water injection methods on a bench scale. One of the challenges of the water injection is to get the water to spray evenly in the reactor in order to properly mix with the syngas. In the previous phase of the project (DE-FE-0012048), we used a gasoline direct injector to inject high pressure water into the reactor. The injector is a solenoid type that operates on 60 VDC. We built an injector driver consisting of a microprocessor and MOSFET solid state relays to pulse the injector as fast as 100 µs. The injectors were installed into the reactors so that tip of the injector was perpendicular to the flow of syngas. This worked well for our smaller test reactors which were 4” in diameter. However, the CFD modeling done by GTI in this project showed that spraying from the side of a larger reactor will not provide efficient mixing and cooling the syngas and the sorbent/catalyst bed. Their suggestion was to get the injector inside the vessel and spray the water in a counter current direction to the syngas. Since the injectors used in the previous project were electronically operated, it meant they would always have to be installed from the side of the reactor in order to leave the solenoid outside of the reactor.

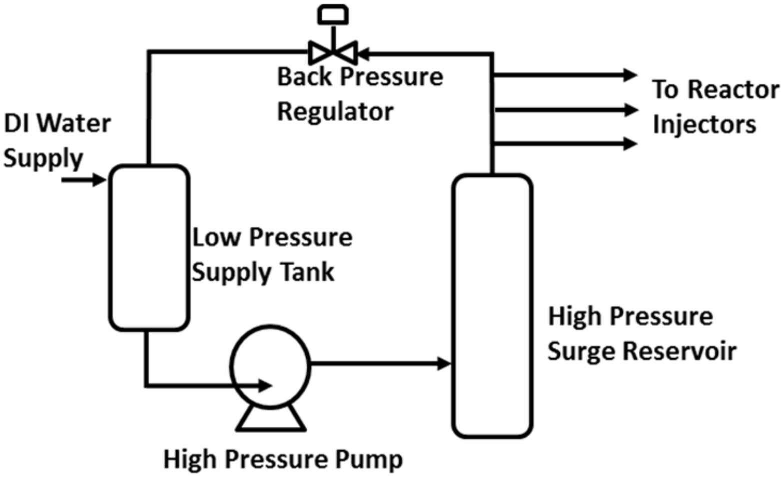


Figure 34. Injector supply setup.

The injector supply will be similar to the diagram shown in Figure 34. DI water is supplied to a low pressure tank where a high pressure piston pump pressurizes the water to >1000 psig. Pressure in the surge reservoir and the injector lines are maintained by a back pressure regulator.

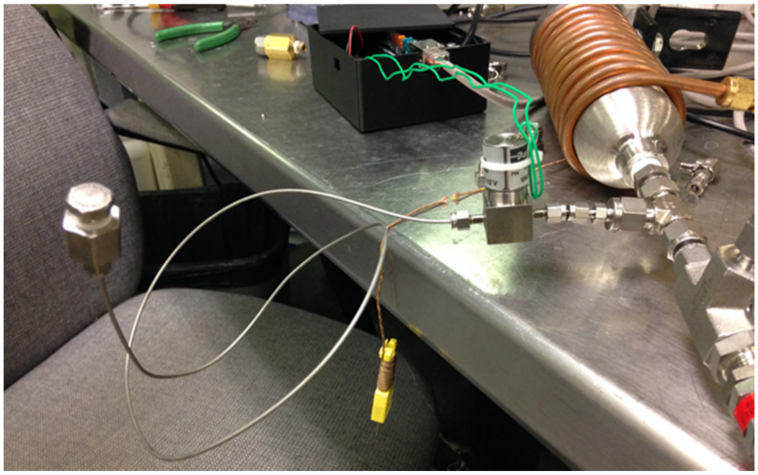


Figure 35. Micro dispensing valve and orifice water injection.

We tested various methods for water injection and upon settling on a design, we bench tested the following setup which involved attaching an orifice of approximately 0.015 in diameter to the end of a 1/16 in line which is attached to the outlet of a micro dispensing valve capable of pressures to 1200 psig. The setup is shown Figure 35. The dispensing valve can cycle as fast as 5 ms and the timing is controlled by the driver electronics developed in previous experiments. When the valve opens, a slug of high pressure liquid is sent to the orifice which atomizes the water. By the duty cycle of the valve, we can accurately and repeatedly control the amount of water injected into the reactor. Shown in Figure 36 is the calibration curve of the amount of water injected based on varying the valve delay and “on” time. Varying the valve “on” time also can control the quality of spray with

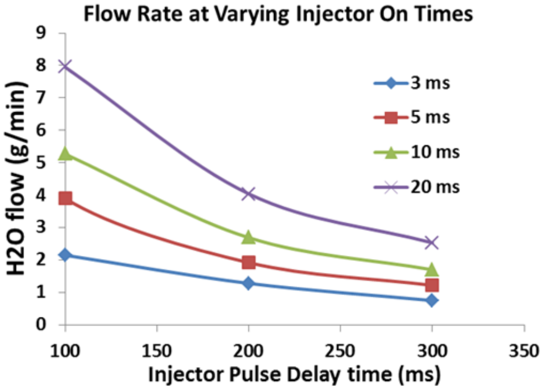


Figure 36. Flow rate calibration for varying valve pulse times.

longer times having better atomization. By increasing the delay time, the amount of water can be decreased to the amount needed. For a 10 SCFM apparatus, we need 5 g/min of water to be injected to the reactor. If 3 orifices are used, they will have to flow 1.7 g/min which this system will be capable of doing. Another advantage of this system is that all mechanical and electrical components are located outside the vessel and away from heat.

The bed is heated by a series of heat tapes to maintain bed temperatures of 180-220 C. The reactor was filled with 20 vol% of Shiftmax 230 LTWGS catalyst and the rest with TDA2015 sorbent. The total volume of the test reactor is 25L. A total of 3 water injectors were inserted at the points. Syngas flows from the bottom of the reactor to the top while sorbent regeneration N_2 flow countercurrent from the top of the reactor to the bottom. The bottom section of the reactor is filled with just sorbent. The second section from the bottom contains half of the total catalysts in a layer sandwiched between two layers of sorbent. A thermocouple was installed in the center of the catalyst layer. The third section from the bottom contains the other half of catalyst homogeneously mixed with sorbent. The fourth section contains only sorbent in order to adsorb the remaining CO_2 that is generated from the WGS sections.

5.8 Task 9. Evaluation of Single Reactor

Figure 37. Adjustable separation screen.

In this task, we evaluated the performance of the single test reactor evaluations.

Adjustable screens were fabricated as shown in Figure 37. The support screens can travel up and down the reactor on three support columns that are welded to the inside of the reactor. Once the desired location is determined, set screws lock the screen in place. This mechanism will allow us to test various injection locations to determine where the ideal placement of the water injection points is. The screens are also used to divided the bed into sections and allow a space for the injected water to vaporize and mix with the crossflowing syngas. We installed the reactor in an existing testing apparatus to flow simulated syngas at flowrates up to 10 SCFM (Figure 38). The position of the 3 water injectors in the reactor is shown in Figure 37 (inset).

The water injection is done via 0.035 in orifice and water is pulsed to it via a micro dispensing solenoid valve as shown in Figure 39. The injection orifice is installed in a fashion so that the spray is countercurrent to the syngas flow. This was done to promote good mixing and vaporization.

Figure 40 shows the bed temperatures during a period of testing. There is a thermocouple in each bed section. The left side of the vertical black line is the bed temperatures during water injection. The inlet steam:CO was fixed at 1 (which is identical to that of NCCC's). Water was injected at a rate to raise the overall steam:CO to 1.5. The right side is also operating at a steam:CO 1.5 but without water injection. On average, the bed temperatures rose approximately 20°C when operating at the same steam:CO without the water injection.

Figure 38. Single bed reactor installed in testing apparatus.

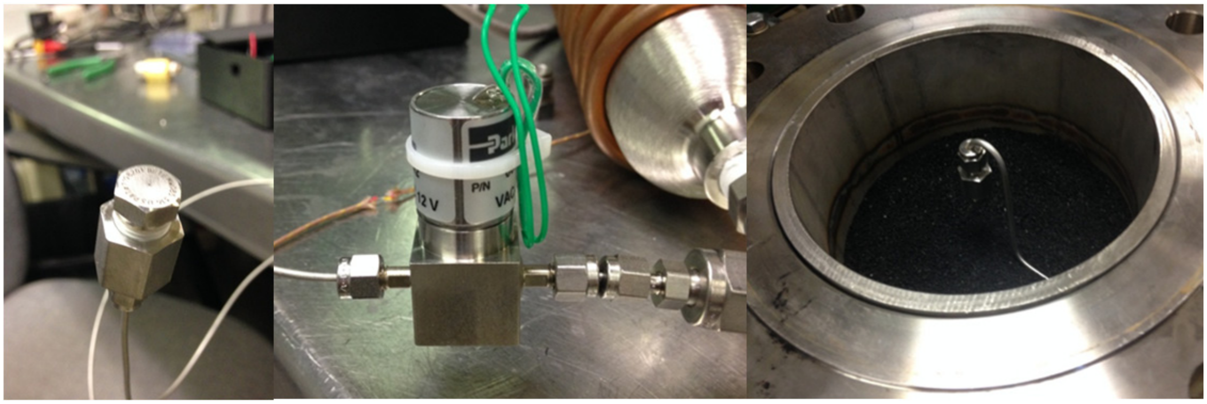


Figure 39. Nozzle detail and installation in reactor

Figure 41 shows the moles of CO that were converted in the bed via WGS. When the bed was operating with the water injection, the amount of CO converted was upwards of 20% more than the CO converted without water injection at the same steam:CO ratio.

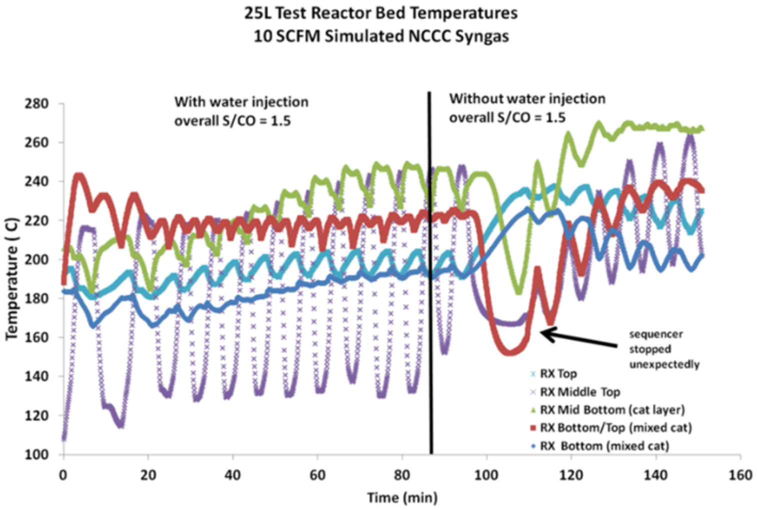


Figure 40. Single reactor bed temperatures.

Figure 42 shows the sorbent CO_2 capacity with and without water injection. On a whole the capacity was slightly lower with water injection. This could be due to the localized decrease in CO_2 partial pressure due to the increase in water vapor near areas of injection.

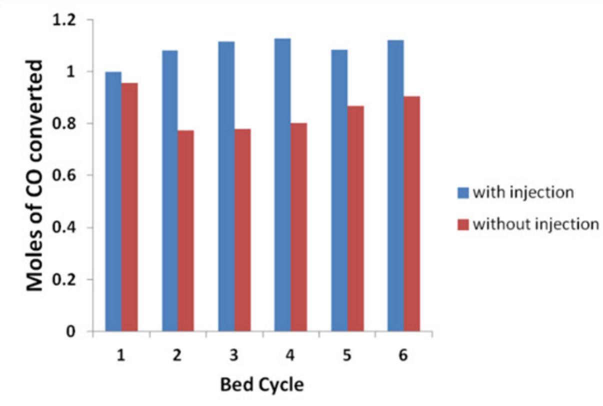


Figure 41. Moles of CO converted.

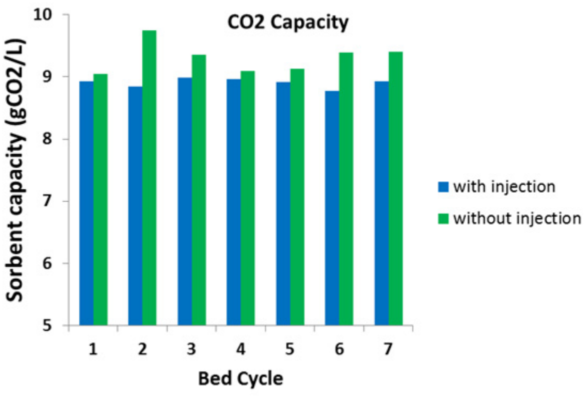


Figure 42. Sorbent capacity.

5.9 Task 10. Reactor Design Revisions

Based on the CFD model development and assessment of heat management options, the advantages (pros) and disadvantages (cons) of the various heat management schemes explored are summarized in Table 7. We observed that radial injection used in previous project (DE-FE0012048) is a poor method particularly for beds of larger diameter. So we picked axial water injection.

Table 7. Heat Management Schemes for the Integrated WGS/CO_2 Separation Sorbent Reactor

Cooling Method	Type	Pro	Con
Jacket	Full/Partial	Full jackets, over partial jackets, perform OK through higher CO conversion. Simple to implement.	Radial quenching, poor temp. distribution, lowest CO conversion
Embedded Tubes	Central	Lower quenching of WGS reaction than jackets	Radial uniformity is low
	Distributed	Best radial heat management, partial tube length within combined WGS/sorbent bed is best.	Three tubes needed for 6” reactor, the number of internal tubes and cost becomes prohibitive when extended to full scale reactors.

Water Injection	Axial (1/2)	Performs similarly to distributed, embedded tubes, and the heat management is excellent. Multiple injectors show favorable T control and operational flexibility.	Tradeoff between hot spots and overcooling, difficult to optimize for single injector option. With multiple injections along axial direction, we get optimal temperature control and flexibility in controlling each zone separately by altering the water injection rate.
	Radial	Easier to implement than axial injection	Radial jet penetration is poor, resulting in quenching and poor radial heat management

We then revised the reactor configuration and explored a second configuration to determine the efficacy of the sorbent/catalyst layer layout on CO conversion. Both the first and the revised configuration consisted of 20 vol% of identical LTWGS catalyst. The two configurations are shown in Figure 43. In configuration 1, half the catalyst resided in the middle of the bed as a solid layer while the other half is equally mixed in the upper and lower parts of the vessel. In configuration 2 (also called as single reactor design revision), half the catalyst resides in a layer in the middle of the reactor while the other half is mixed in the top portion of the vessel only.

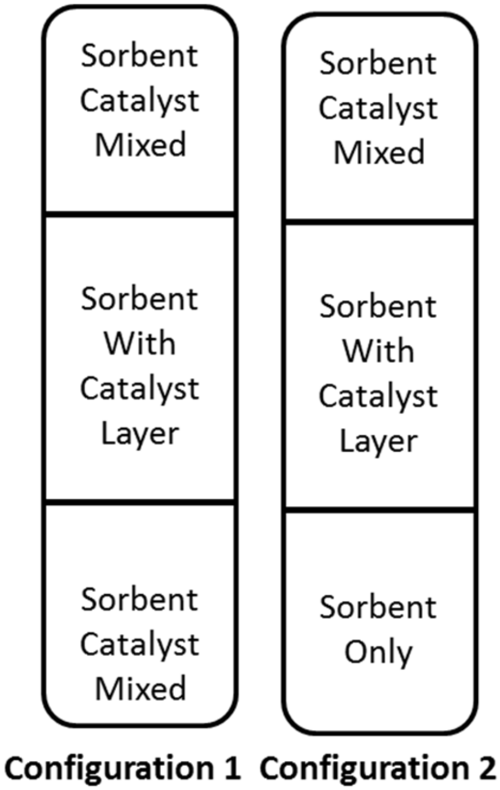


Figure 43. Two tested bed configurations.

5.10 Task 11. Fabrication of Single Reactor Revisions

We fabricated the new reactor configuration by having the three segments as shown in Figure 43 and had the single bed reactors hooked up to the bench-scale test setup shown in Figure 38.

5.11 Task 12. Evaluation of Single Reactor Revisions

We tested the two bed configurations with syngas flow from both directions i.e., from top-to-bottom and bottom-to-top. Both configurations were tested using the same inlet CO concentrations and Steam to CO ratio of 1.2. Figure 44 shows a difference in the total CO conversion. Using configuration 1, the CO conversion yielded on average 3.5% more CO converted than configuration 2.

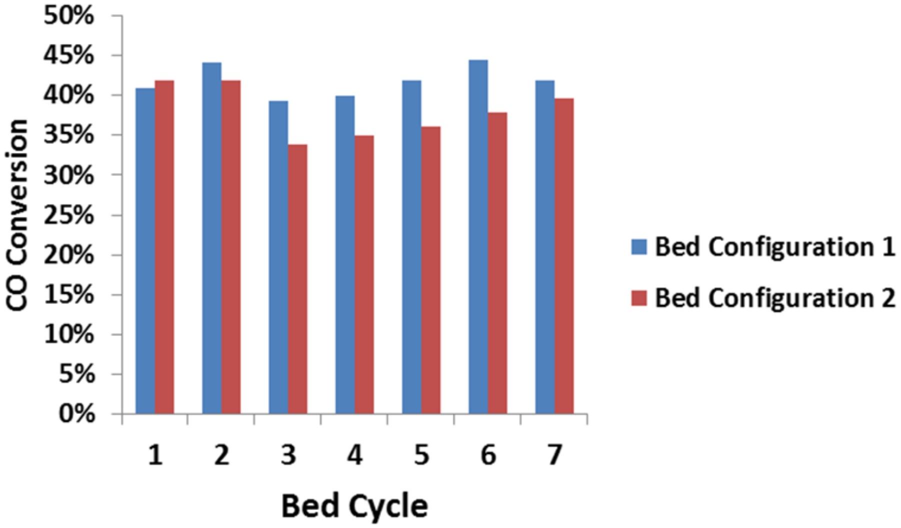


Figure 44. CO conversion

5.12 Task 14. Critical Design Review

Before finalizing the Test Unit's P&IDs, we completed a critical design review, which included a thorough Process Hazard Analysis (PHA) was performed in conjunction with engineers from Sinopec, Southern Company operators of the Power Systems Demonstration Facility (PSDF) at the National Carbon Capture Center and operators of other potential demonstration sites. The PHA ensured that 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. A detailed Failure Modes and Effects Analysis (FMEA) was carried out by TDA to identify safety vulnerabilities and correct them in the design.

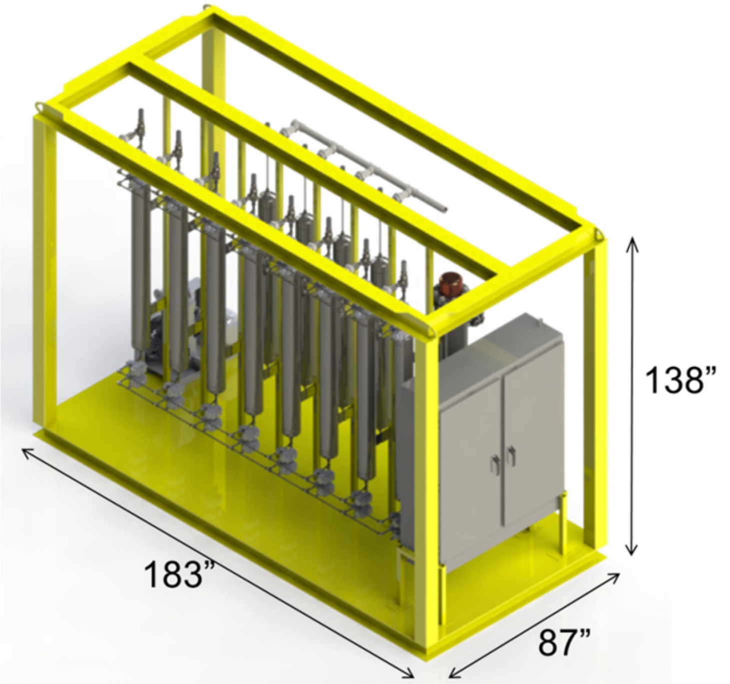


Figure 45.3-D layout of the 10 scfm integrated WGS and CO_2 capture field test unit.

5.12.1 Facilities Requirements

The 3-D sketch for the overall system is shown in Figure 45. The 10 scfm skid included limited gas conditioning capabilities eliminating the need for a separate gas processing skid. The facilities requirements for the 10 scfm skid are summarized in Table 8.

Table 8. Facilities requirements for the 10 scfm integrated WGS and CO_2 capture skid.

Utility Requirements			
Power		**Syngas Outlet**	
Voltage	480	Flow, scfm	9.0
Max Current (Startup), Amps	102	Pressure, psig	7.0
Normal Current, Amps	36	Temperature, °F	390
Syngas Supply		Connection Type	Swagelok Compression, 3/4 in
Quality	Desulfurized, Unshifted	**CO2 Waste Outlet**	
Nominal Flow, lb/hr	50.0	Flow, scfm	9.0
Max Flow, lb/hr	60.0	Pressure, psig	7.0
Temperature, °F	400	Temperature, °F	390
Pressure, psig	200	Connection Type	Swagelok Compression, 3/4 in
Connection Type	Swagelok Compression, 1/2 in	**Relief Vent**	
Cooling Water Supply		Max Flow, scfm	1043
Flow, gpm	10.9	Connection Type	2in pipe, 150# flange
Temperature °F	<95	**Condensate Return**	
Pressure, psig	60	Flow, gph	2.4
Connection Type	Swagelok Compression,1in	Pressure, psig	Amb
Cooling Water Return		Temperature, °F	Amb
Flow, gpm	10.9	Connection Type	Swagelok Compression, 1/2 in
Temperature °F	<106	**Nitrogen**	
Pressure, psig	35	Max Flow, scfm	40 (during Skid Heat up Only)
Connection Type	Swagelok Compression, 1 in	Nominal Flow, scfm	2.0
Steam		Pressure, psig	350
Flow, lb/hr	15.1	Connection Type	Swagelok Compression, 1/2 in
Pressure, psig	325	**Instrument Air (may use N2 if necessary)**	
Temperature, °F	600	Flow, scfm	5.0
Connection Type	Swagelok Compression, 1/2 in	Pressure, psig	100
		Connection Type	Swagelok Compression, 1/2 in
		Municipal Water	
		Flow, gph	0.5
		Pressure, psig	<100
		Connection Type	Swagelok Compression, 1/4 in

5.13 Task 15. Fabrication of Field Test Unit

For the fabrication of the field test unit, we used the vendor Springs Fab located in Colorado Springs, approximately 90 miles from TDA's office for the fabrication of the skid and the vessels. We had worked with Springs Fab in the past and felt confident in their abilities. We had a kickoff meeting on Aug 12, 2016 to finalize and approve the drawings for the skid and vessels. Fabrication began shortly after this meeting. On October 7, 2016 we visited Springs Fab to inspect the fabrication progress. We inspected one vessel before the final welding took place to ensure that the injector inserts we had designed would work.

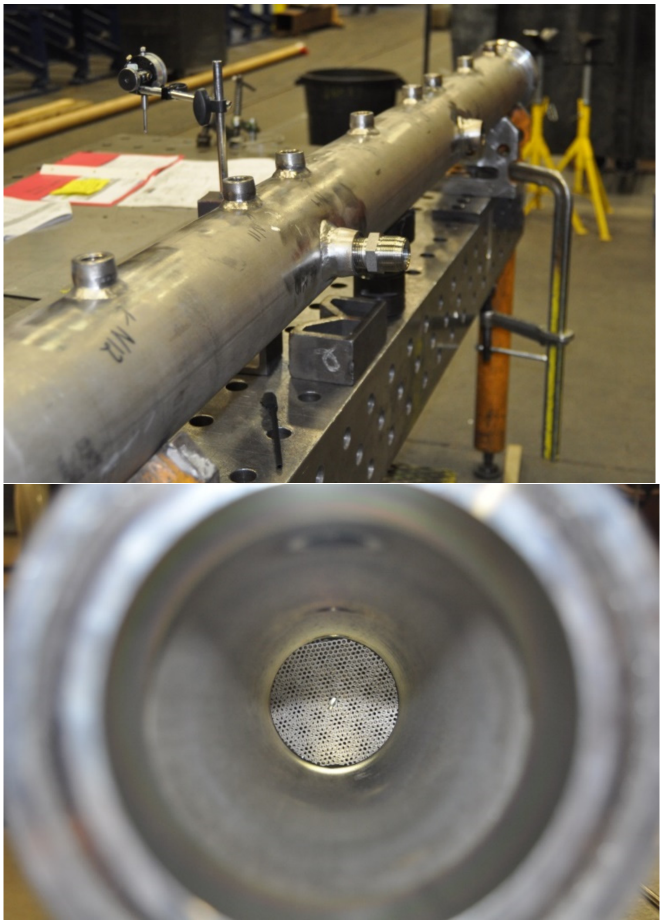


Figure 46. Vessel during fabrication (top), vessel insert during test for fit (bottom)

Figure 46 shows one of the fully instrumented vessels during the fabrication process. The insert was test fitted to the reactor to determine the dimensions needed for it to fully slide down the length of the reactor. After test fitting the insert, the remaining vessels were fabricated.

On October 26, 2016, the skid fabrication was completed and powder coated. All the vessels other than the reactors were mounted to the skid (Figure 47). At the beginning of November 2016, the assembled skid was transported to a metal machine shop located 3 miles from TDA. Here we performed all the plumbing and wiring.

Figure 47. Skid frame progress and vessel mounting.

Fabrication of Electrical Control Panel: The fabrication of the electrical control panel was carried out by TDA at our Wheat Ridge, CO shop. The system control back-panel is the hardware interface between the provided plant power at 480 VAC, 125 amperes, 3-phase power and the data acquisition hardware required to control system function, collect system data, and provide safety features protecting both operation personnel and system/plant protection. Plant power will tie into a 125 ampere C1D2 disconnect, circuit breaker, knife switch (not shown, as it is external on the main skid) and then tie into the distribution blocks (shown top right in Figure 48).

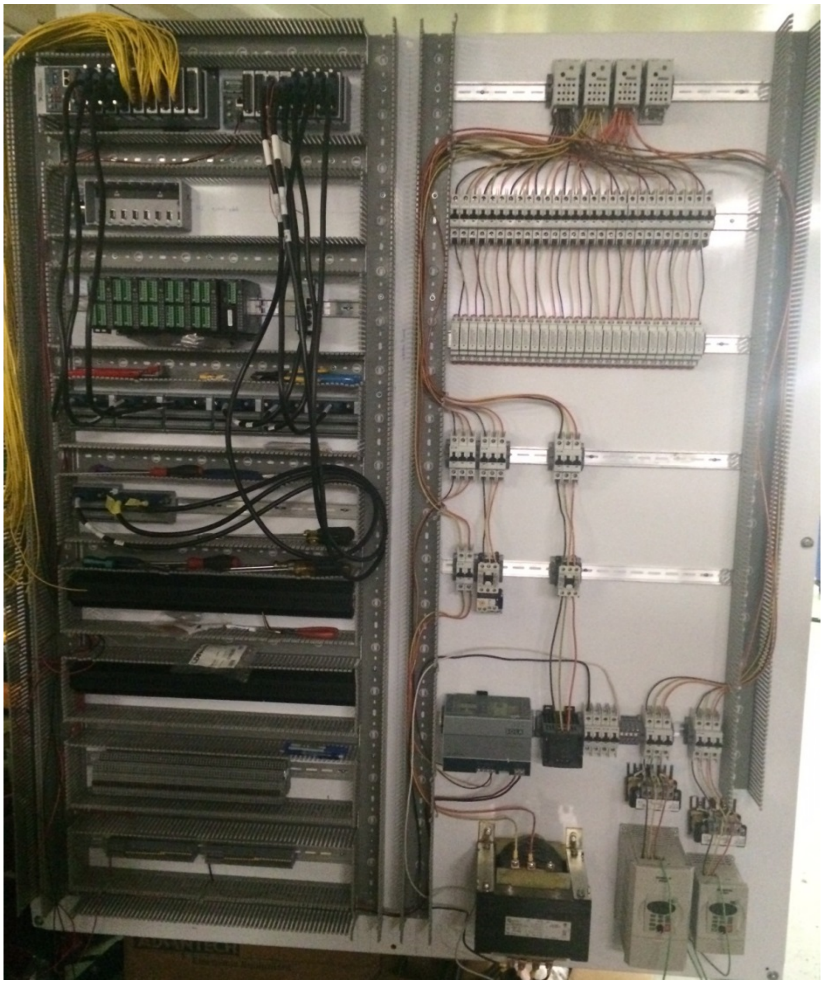


Figure 48. Electrical back panel fabrication in process

The 3ϕ power is distributed to an array of circuit breakers, 960 watt, 24VDC power supply, VFD controllers, 480-120VAC transformer, and contactors for heater control, system heaters and pump control. The 24VDC control voltage is transmitted to the low voltage side of the panel. The system control is managed by National Instrument cDAQ hardware. LabVIEW software is a system-design platform and development environment for a visual programming language completed and tested in house by resident engineers. NI cDAQ-9133 embedded controller and cDAQ-9188 backplanes are populated with NI modules for command and control of the various instruments required in this system. NI modules including NI-9208 current input, NI-9213 thermocouple, NI-9265 current output, NI-9476 sourcing digital output, NI-9425 24V sinking digital input and NI-9477 5-60V sinking digital output are used in this data acquisition scheme. 24VDC is the main control voltage and is distributed from terminal block arrays to fuse blocks and then to relays, NI Module excitation power, Watlow EZ-Zone modules RMHA-1111-AAAA, RMHA-11CC-AAAA, RMEA-CCCC-AAAA, RMLA-55JJ-AAAA and RMAA-A3AA-AAAA, Ethernet network switch power, SSR on/off power, Advantech Touchscreen Monitor, Flow control valves, Pressure control valves, Level sensors (both high and low), Flow meters, Flow switch, Capacitance level transmitter, and Pressure transducers.

120VAC power is provided through a 5000VA Transformer and distributed to 120 VAC devices from the 120VAC terminal block array on the high voltage side of the back-plane. The product stream analyzer, Z-Purge, and system lighting is provided 120VAC power from this terminal block array.

Once the skid arrived from the fabricators, TDA began the plumbing and assembly of the demonstration unit. The first step of the assembly was plumbing the upper and lower valve manifolds. Figure 49 shows how all 40 valves were assembled and mounted in ways to allow for flexing during heat up and cool down.

We worked with GTI to complete the fabrication of the field test unit, including the plumbing, electrical, heat trace and insulation of the sample system selection valves. GTI also procured the WGS shift catalyst from Clariant for use in the field test unit. Figure 50 shows the 20 valves that were used to simultaneously sample different sampling points throughout the system to two different analyzers.

We chose a MKS tunable spectrometer to measure the CO_2, CO and other hydrocarbons. We have used this model instrument in a previous system involving syngas with high success and accuracy. The analyzer cannot analyze H_2 or other diatomic gases (N_2, etc), therefore a separate H_2 analyzer was also installed. The two can work together to give a complete gas analysis for every stream in the system. Two sample chillers and water knockouts were also installed between the valves and the analyzer to eliminate condensed water from entering the analyzer.


Figure 49. Upper (top) and lower (bottom) valves and manifolds.

The mineral insulated (MI) heating cable installation was also completed. Each sorbent reactor, LTWGS reactor, desulfurizer and accumulator vessels have mineral insulated heating cable installed on them to maintain process temperatures (Figure 51). MI cable is tolerant of the high temperatures required by the system while being Class 1 Div 2 electrically compliant. All process lines were also heat traced with MI cable.

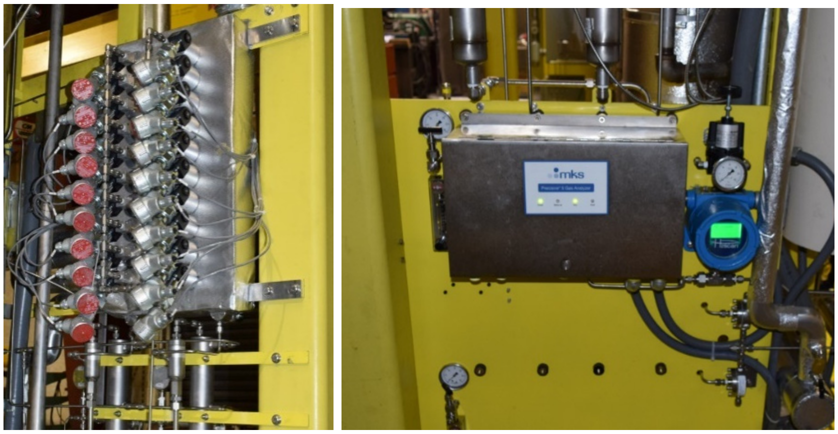


Figure 50. Sample system selection valves (left), analyzers (right).

The system was hydrostatically leak checked using a high-pressure pump with DI water. All the lines and vessels were filled with DI water and pressurized to 600 psig and left for 30 minutes. The pressure was checked again to ensure no leaks were present. If the pressure dropped, the lines and fittings were inspected and tightened if necessary and the test was performed over again until no drop in pressure was observed.

After the system was deemed leak tight, the insulation was installed over all the heat traced vessels and lines. Mineral wool was used due to its high temperature capabilities. The vessels were covered in 3 in thick mineral wool while the smaller process lines received 1.5 in thick insulation. The thickness of insulation was chosen to not only prevent the outer surfaces from being a burn hazard but also to allow us to use much less powerful MI cables to maintain process temperature. The insulation was then covered with aluminum sheathing to keep moisture from penetrating into the insulation. All seams were caulked with silicon to further facilitate in keeping water out. Removable fiberglass jackets were

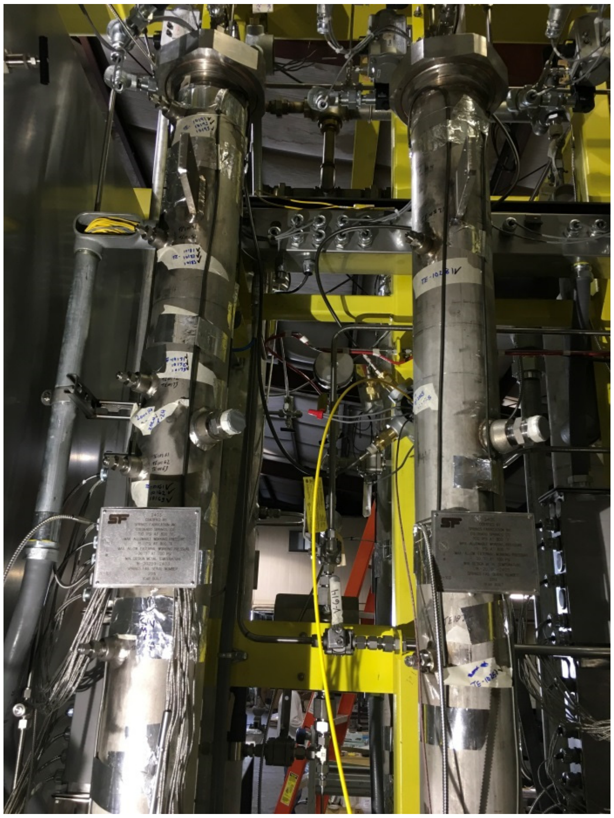


Figure 51. MI cable installed on reactor

Figure 52. Picture of the 10 cfm field test unit after completion with the insulation.

made for the top and bottoms of the sorbent reactors to facilitate in their removal so that we can load and unload the reactors when necessary.

Figure 52 shows the completed test unit after insulation and aluminum sheathing was completed. We were then able to progress to the system shake down testing before shipping it to the first testing location.

5.14 Task 16, 19 Shakedown Testing of Integrated Skid

Once the insulation was finished, the system was powered with 480V power and every piece of equipment was tested and tuned. Both compressors were turned on to verify that their VFD controls were operating and programmed correctly. Every valve was actuated several times to verify that it was opening and closing correctly

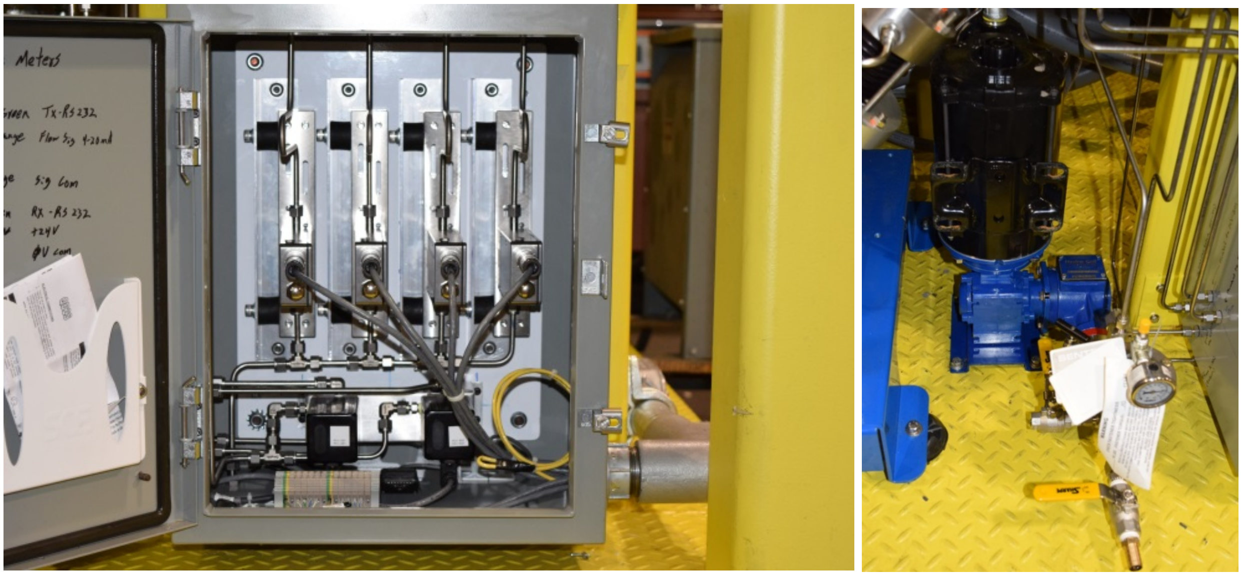


Figure 53. Water injection flow meters (left), high pressure water pump and pulse dampener (right).

The high-pressure water injection system was thoroughly vetted by filling the system with DI water and operating the high-pressure diaphragm pump (Figure 53). A high-pressure pulse dampener was installed on the outlet of the pump to reduce the pressure spikes and pulsing flow from the diaphragm pump. The dampener consists of a bladder on one end and the process fluid on the other. The bladder was charged with 800 psig nitrogen. The gas bladder compresses during pump strokes and expands when the pump refills to help reduce pulsing. The system was brought to pressure and the solenoids were then operated with different duty cycles and two different inlet pressures. The sprayed water was collected in a graduated cylinder for exactly 2 mins to calculate actual water being sprayed. It was then compared to the mass flow meters indicated flow rate. Both values matched, verifying the flow meters were measuring the correct flow.

Figure 54 shows how we control the water flow by altering the duty cycle of the injection valves. The valves will operate a max differential pressure of 1000 psig but normal differential pressure will be 500 psig. As shown, the flowrate can be precisely altered by changing the duty cycle of the valve. Below 0.5% duty cycle, the valve is unable to open and close correctly. The required flow rate for a single injector is 3 mL/min so we are able to control in this range for both differential pressures.

The flow meters were calibrated to produce a smooth output reading despite the pulsating flow. They have the ability to apply filters to smooth outlying data points, thereby producing a clean and consistent reading.

All the MI cable heat trace zones were turned on to auto tune the PID controllers. All zones reached their given set points without incident.

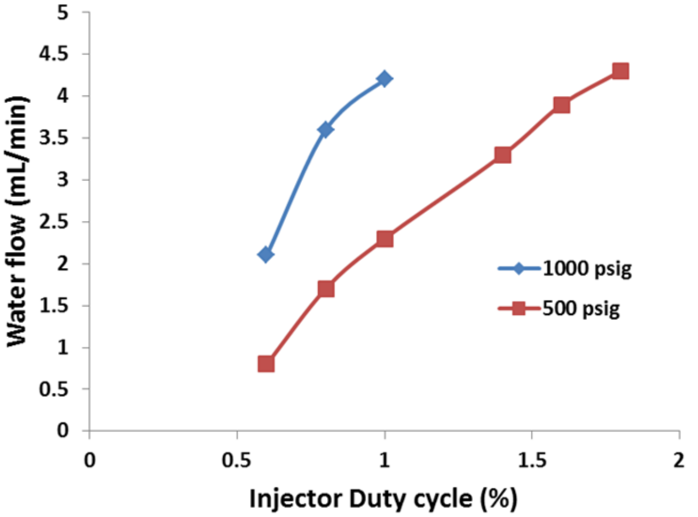


Figure 54. Single injector flow rates at 500 and 1000 psig inlet.

The inlet compressor was turned on and the system was pressurized with air to 400 psig to ensure everything worked as it should. This was the maximum outlet pressure the compressor could achieve since it's designed for 200 psig inlet and the compressed air was only 100 psig.
The flow control valves were tuned so that they closed and opened completely according to their given signals. The pressure control valves were operated according to their respective ranges and were found to be working as expected. The process flow meters were found to be operative. The main process heater was briefly turned on and found to heat up; without significant flow, we didn't want to overheat it.

After shaking down the system as much as possible at the fabrication location, the system was wrapped and shipped to Praxair on July 31, 2017. The unit was installed at their location (Figure 55)

Figure 55. TDA's 10 cfm field unit installed at Praxair's testing location.

Once installed, TDA personnel traveled to Tonawanda, New York in order to fill the reactors with sorbent and catalyst and perform additional shakedown testing that couldn't be accomplished at the fabrication site.

After deployment of the unit at site (Figure 55), each reactor was individually unbolted from the center support for loading with catalyst and sorbent (Figure 56). A custom pivot arm was used to support the reactor and allow it to swing away from the frame in order to gain clearance to load the reactor (Figure 56, left). A spacer and set of screens were strategically placed at each injector port. Precise amounts of catalyst and sorbent was loaded into each section of the reactors.

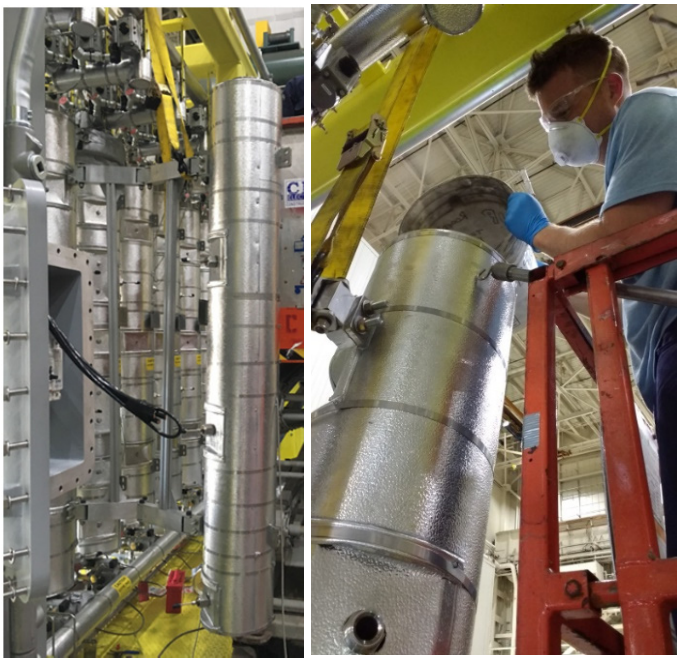


Figure 56. Reactors being loaded with catalyst and sorbent.

The location of water injectors/distances, spacer width and sorbent bed lengths for each reactor are shown in Figure 57 left, while Figure 57 right shows the sorbent and catalyst distributions and weights in various sections of the reactor. During Budget Period 1, GTI performed CFD modeling work pertaining to direct water injection into a 6-inch reactor using the two

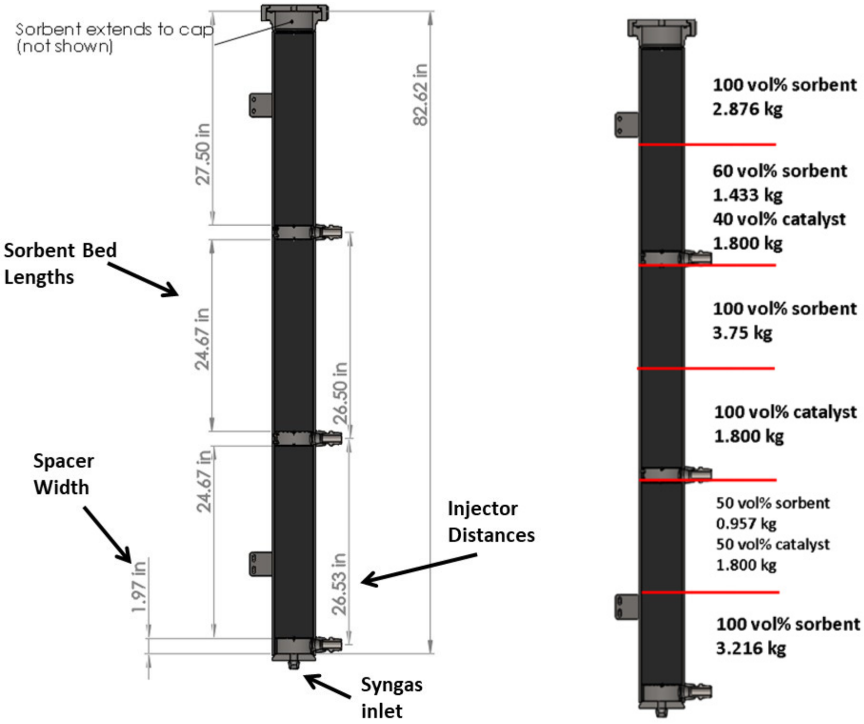


Figure 57. Location of injectors (left); sorbent and catalyst loading (right).

configurations (A & B) shown in Figure 25. Two injection methods, axial and radial, were considered using one 1/64” diameter orifice/nozzle. In axial injection, water sprayed co-current with syngas flow, with nozzle positioned at top of mixed sorbent/catalyst region ~ 10” downstream of vessel top. The purpose was to inject water close to the hottest portion of shift reaction and for the spray to have adequate coverage of the reactor bed. In radial injection water sprayed from the side of the vessel and positioned above the catalyst only layer, with an intention to have sensible heating of spray prior to contact with heat from shift reaction. The goal in this mode was to achieve lateral penetration of spray jet into the gap. The axial injection of water resulted in uniform cooling pattern as expected for embedded tubes in the bed. Radial injection resulted in partial quenching of shift reaction with liquid water streaming along one side and velocity contours of water rates causing overcooling or undercooling of the bed. However, with the small reactors used in the 10 cfm field unit, injections from the radial walls are still near the hottest zone in the reactor.

There were delays in the availability of the Praxair’s Oxygen transport membrane modules (OTM) for the field tests at Praxair. Even though OTM modules are not needed for TDA’s tests, the Praxair field test was planned to be an integrated test with Praxair’s OTM modules. Therefore, these tests were re-scheduled for May of 2018.

5.15 Task 20. Field Testing at Praxair

Once Praxair’s OTM unit was operational, TDA personnel traveled there to begin initial testing. Several trips were made between April and June, 2018.

We reduced the catalyst in the LTWGS reactor and all of the sorbent reactors by feeding in approximately 2% H_2 mixed with nitrogen in order to prevent a rapid temperature increase in the sorbent due to reduction of the metals in the catalyst. This process took several days finish. We worked with Praxair’s safety department to verify everything was in compliance with their site safety requirements in order to start running.

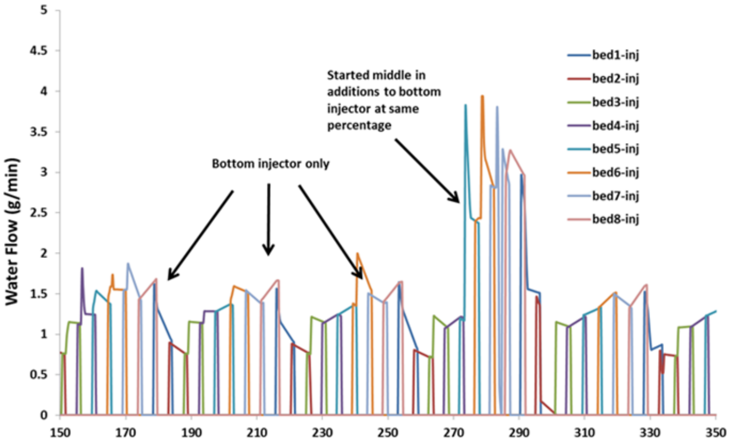


Figure 58. Water injection flow rate flow all beds.

Syngas was first introduced into the system on May 29, 2018. This was to test Praxair’s shutdown system to ensure if our system had an alarm, their system would divert the syngas to a vent location with little to no impact on the pressure of their panel.

The water injection system was tested. The system showed that it was able to precisely and consistently control the addition of water down to 1 g/min. Figure 58 shows the flow rate of water at a continuous valve opening percentage for all the bottom injectors. The amount of water that is injected is determined by the cycle time of the injection valve. As shown, the amount of water that is injected into each bed is approximately 1.2 g/min +/- 0.3 g/min. At the 275 min mark, the middle injector was turned on for each bed while the bottom injector remained on. The flow rate doubled. This shows that the injection system is able to control the water flow rate at a very precise level.

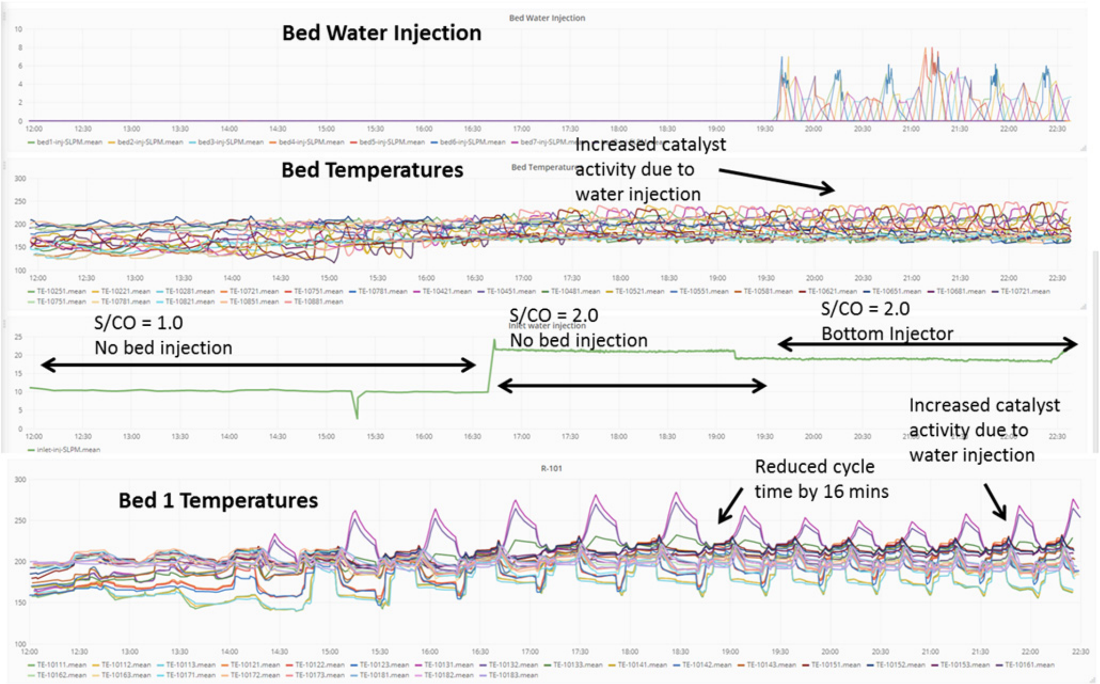


Figure 59. Bed temperature data. Note: S/CO here indicates the Steam to CO ratio

The first significant run using Praxair syngas came on June 6, 2018. The inlet syngas was cooled and the water was condensed out. It then was compressed to 300 psig. Water was reintroduced to bring it back to the same composition (10 vol%). The data in Figure 59 shows a period of operation where there was no bed injection but using the inlet water for shift at a steam:CO of 1.0. The inlet water concentration was then increased to a steam:CO of 2.0. Then the bottom injector of all the beds was turned on and the inlet water was reduced slightly to maintain an overall steam:CO of 2.0. The data in Figure 59 spans a period of 10.5 hours. Bed 1 has a full suite of thermocouples with 9 3-point profile probes evenly spaced along the bed. As observed, the bed began to increase in temperature with just the inlet water as the reactant and no cooling via injection. Once the inlet was increased to a steam:CO of 2.0, the temperature of the outlet of the mixed catalyst and sorbent zone began to increase rapidly to over 280 C. At this point, the cycle time was dropped to see what impact it had on the CO_2 capture percentage. This caused the temperature in the catalyst zone to drop due to less gas being processed during the adsorption step. Shortly after the step time change, we began injecting water into the bottom injector of all the beds. This caused the temperature in the catalyst zone to begin to rise again, indicating that more CO was being converted than before. Unfortunately, a drain quit working and liquid water got into the system and had to be temporarily shut down. This shows that even injecting a minor portion of the full amount of water can increase WGS activity and influence bed temperature.

Figure 60 shows the gas compositions of the inlet, outlet and regeneration streams as well as the flow rates. There is only one gas measurement device on the system, so we cycled through different sampling points throughout the testing period. The inlet to the beds contained 10% CO while the outlet of the beds showed 0% CO, indicating that nearly all the CO was being shifted inside the reactors. The amount of the CO_2 in the outlet stream is high at an average of 14%.

The inlet flow was changed from 8.7 SCFM to 4.75 SCFM during the run and the CO_2 in the outlet didn't change. This would indicate the cycle time needs to be further reduced to prevent CO_2 breakthrough.

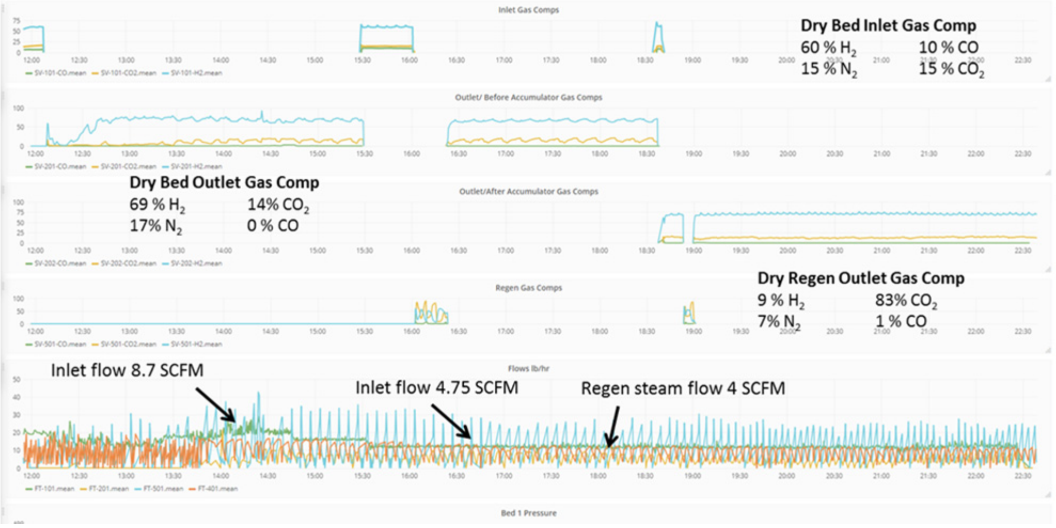


Figure 60. Gas compositions during 300 psig inlet pressure operation.

The regeneration stream contains an average of 9% H_2 and about 1% CO. This high amount of H_2 is due to the fact the co-depressurization or recycle was not in operation during this test. Once this part of the system is running, it would evacuate the residual gas in the reactor before regeneration and pump it back to the inlet. This will decrease the amount of H_2 and CO that is being wasted in the regen stream.

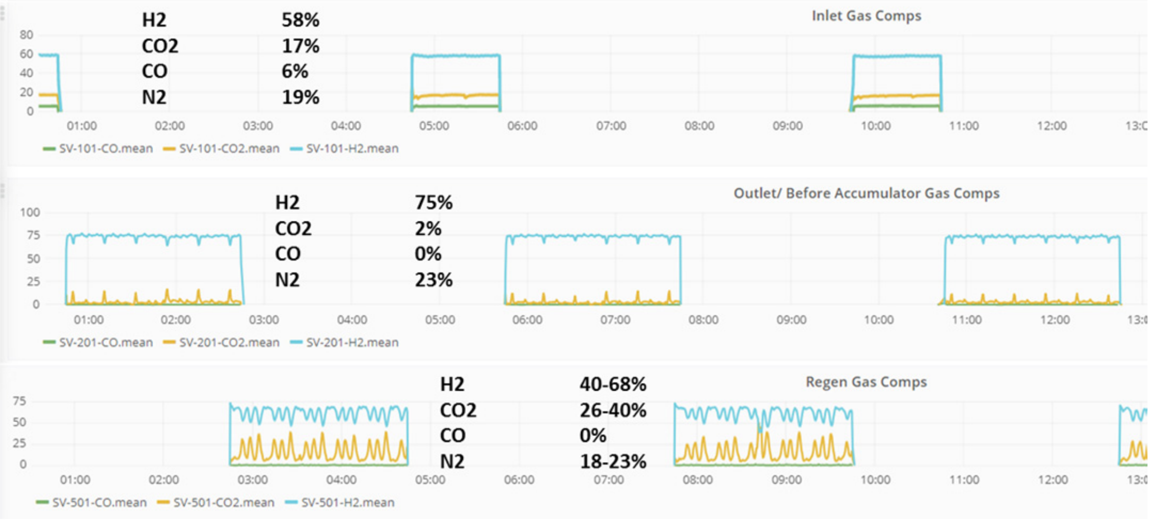


Figure 61. 100 psig syngas operation

As stated earlier, a level switch mal-functioned, preventing condensate from being pumped out of the system. This resulted in water getting into the compressor inlet, which damaged it. The compressor was bypassed and the system ran at Praxair's inlet pressure (100 psig) for an additional 48 hrs until Praxair had a shutdown of their system. The level switch problem was fixed, after which the condensate system was verified to be working as designed.

Figure 61 shows the gas compositions during this period. The inlet flow was maxed at 3.8 SCFM due to the reduced inlet pressure and the pressure drop through the system. The average carbon capture during this time period was 91%. The average outlet CO percentage in both the product syngas and regen stream was below the minimum detection limit of the analyzer which is 0.1%. This indicates a very high rate of conversion (near 100%) that occurred in the sorbent beds. The flowrate of syngas was low enough that bed water injection was unnecessary as the temperature of the bed remained relatively unchanged.

The test run from May 29, 2018 through June 30, 2018 was Field Test #1. The system was unable to be restarted in time for the end of Praxair's run on this panel.

We traveled to Praxair (now Linde) to repair and modify the apparatus and start the Campaign #2 testing, using both bottled gases (CO_2 in N_2 mixtures) as well as syngas generated by Linde's OTM panel. These tests were carried out between September 14 and 27, 2020.

5.16 Task 21. Field Test at Praxair #2

In the first week of the second test campaign, we added 2 mass flow controllers in order to flow bottled nitrogen and carbon dioxide gases into the system so that we can carry out additional tests while the OTM membrane is down. We replaced the small tee style filters with larger filters in order to run longer between clean outs, as sorbent dust is prevalent in PSA systems. We started the system and began running on the CO_2/ N_2 mixture while their OTM was heating up. We ran a total of 57 hours under CO_2/N_2 mixtures, demonstrating CO_2 capture between 63 to 100%.

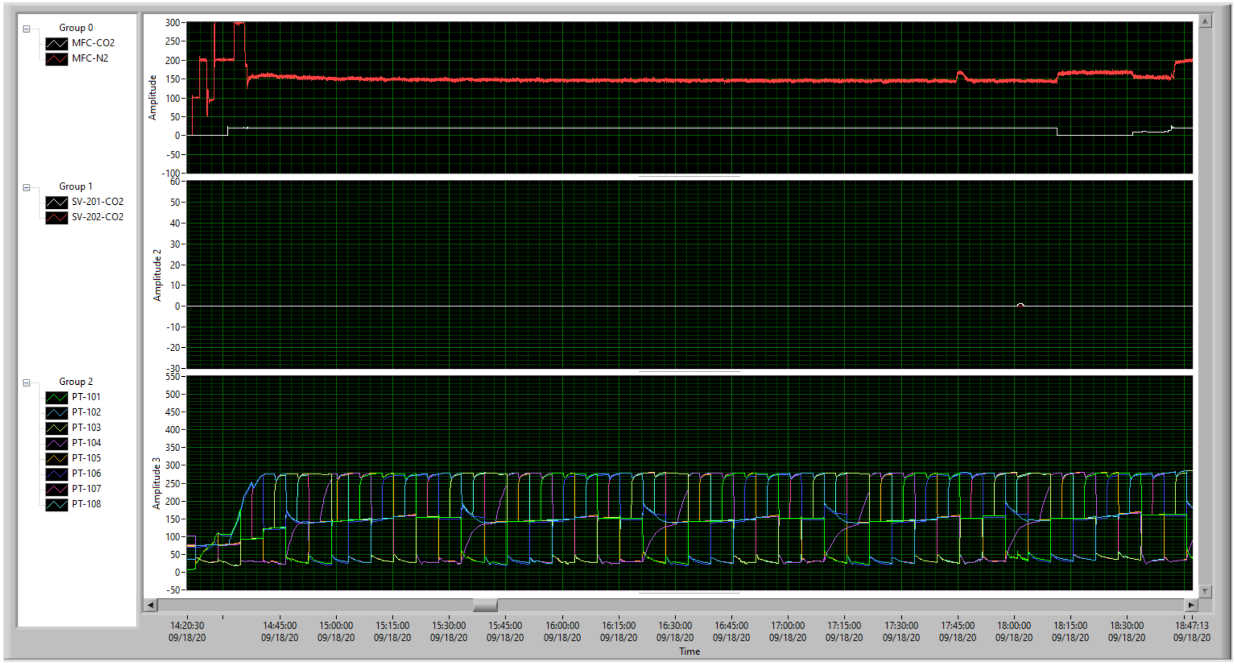


Figure 62. Campaign # 2: Test #1 - 4 hours test 09/18/2020 – 14:45 to 18:45 hours.

Figure 62 shows the result from the Test #1, which ran for 4 hours on 09/18/2020 between 14:45 to 18:45 hours (a total of 4 hours). The feed flow was 20 slpm CO_2 and 150 slpm N_2 at an adsorption pressure of 180 to 275 psig with desorption being carried out between 25 and 40 psig. We used a full cycle time of 48 min in these tests and did not observe any CO_2 in the high-pressure syngas product, providing 100% CO_2 capture at CO_2 removal rates of 56.5 kg CO_2/day.

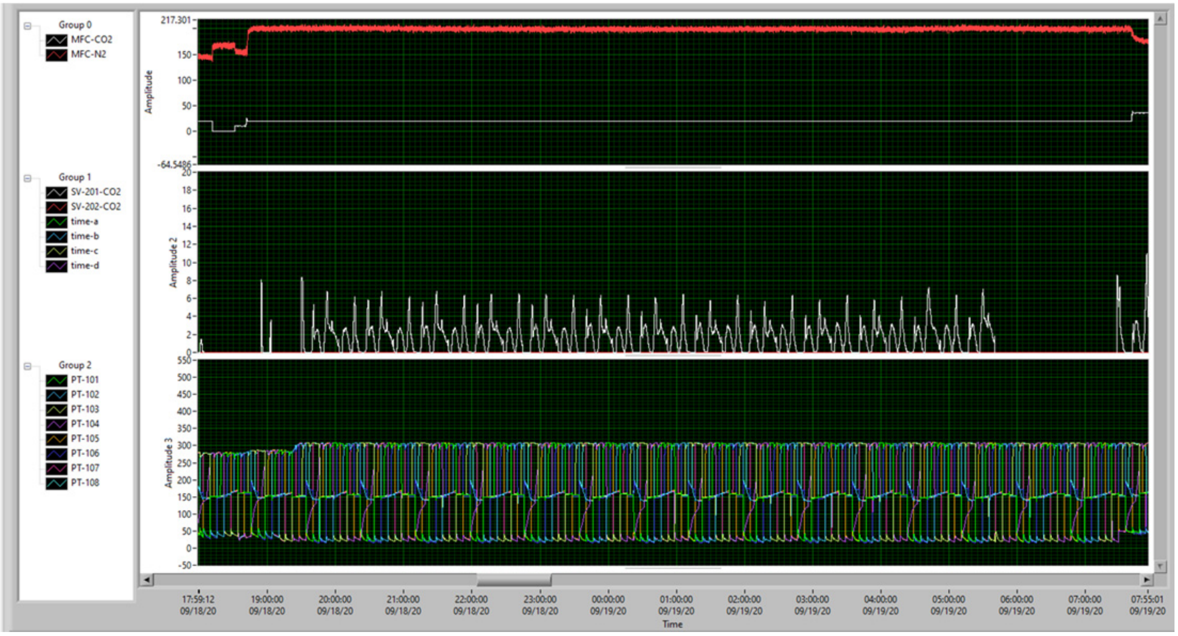


Figure 63. Campaign # 2: Test #2 - 12 hours test 09/18/2020 19:30 to 09/19/2020 7:30.

Figure 63 shows the result from the Test #2, which ran for 12 hours between 09/18/2020 19:30 to 09/19/2020 07:30 hours (a total of 12 hours). The feed flow was 20 slpm CO_2 and 200 slpm N_2 at an adsorption pressure of 280 to 300 psig with desorption being carried out at 20 psig. We used a full cycle time of 48 min in these tests and observed about 2.5% CO_2 by vol. in the high pressure syngas product, providing 80% CO_2 capture at CO_2 removal rates of 49.5 kg CO_2/day.

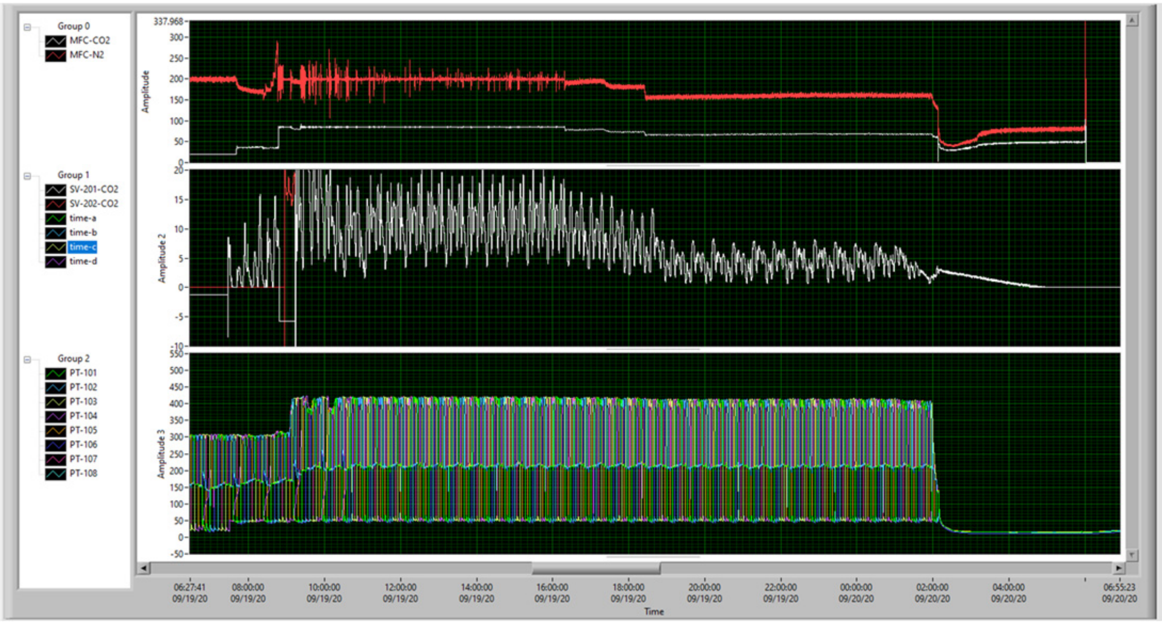


Figure 64. Campaign # 2: Test #3 – 18.5 hours test 09/19/2020 07:30 to 09/20/2020 02:00.

Figure 64 shows the result from the Test #3, which ran for 18.5 hours between 09/19/2020 07:30 to 09/20/2020 02:00 hours (a total of 18.5 hours). The feed flow was varied between 20 to 85 slpm CO_2 and 150 to 200 slpm N_2 at an adsorption pressure of 300 to 400 psig with desorption being carried out at 50 psig. We used full cycle times between 32 and 48 minutes in these tests and observed between 0 and 15% CO_2 by vol. in the high-pressure syngas product, providing between 63.1 and 100% CO_2 capture at CO_2 removal rates between 56.5 and 170.8 kg CO_2/day.

Figure 65. Campaign # 2: Test #4 – 18.5 hours tests 09/22/2020 15:30 to 09/23/2020 10:00.

Figure 65 shows the result from the Test #4, which ran for 18.5 hours between 09/22/2020 15:30 to 09/23/2020 10:00 hours (a total of 18.5 hours). The feed flow was varied between 10 to 40 slpm CO_2 and 150 to 190 slpm N_2 at an adsorption pressure of 300 to 325 psig with desorption being carried out at 50 psig. We used full cycle times between 16 and 32 minutes in these tests and observed between 0 and 4% CO_2 by vol. in the high-pressure syngas product, providing between 80 and 100% CO_2 capture at CO_2 removal rates between 28.3 and 213.1 kg CO_2/day.

After Praxair's OTM panel was in operation, we began flowing syngas to the system. We compressed it to 350 psig for the feed pressure and desorption pressure was set at 50 psig using steam. The inlet flow rate was estimated to be approximately 250 SLPM and the regen flow rate was set at 100 SLPM.

We ran for a total of 68 hours on syngas before an issue with condensate collection on Linde's OTM panel forced a shutdown. The average inlet compositions were as follows: 75% H_2, 17% CO_2 and 8% CO (Figure 66). The majority of the water in the inlet was condensed in order to compress the syngas. We did not carry out any WGS prior to the gas entering the integrated sorbent/catalyst beds. We used water injection to provide the necessary water for the WGS reaction occurring in the sorbent beds.

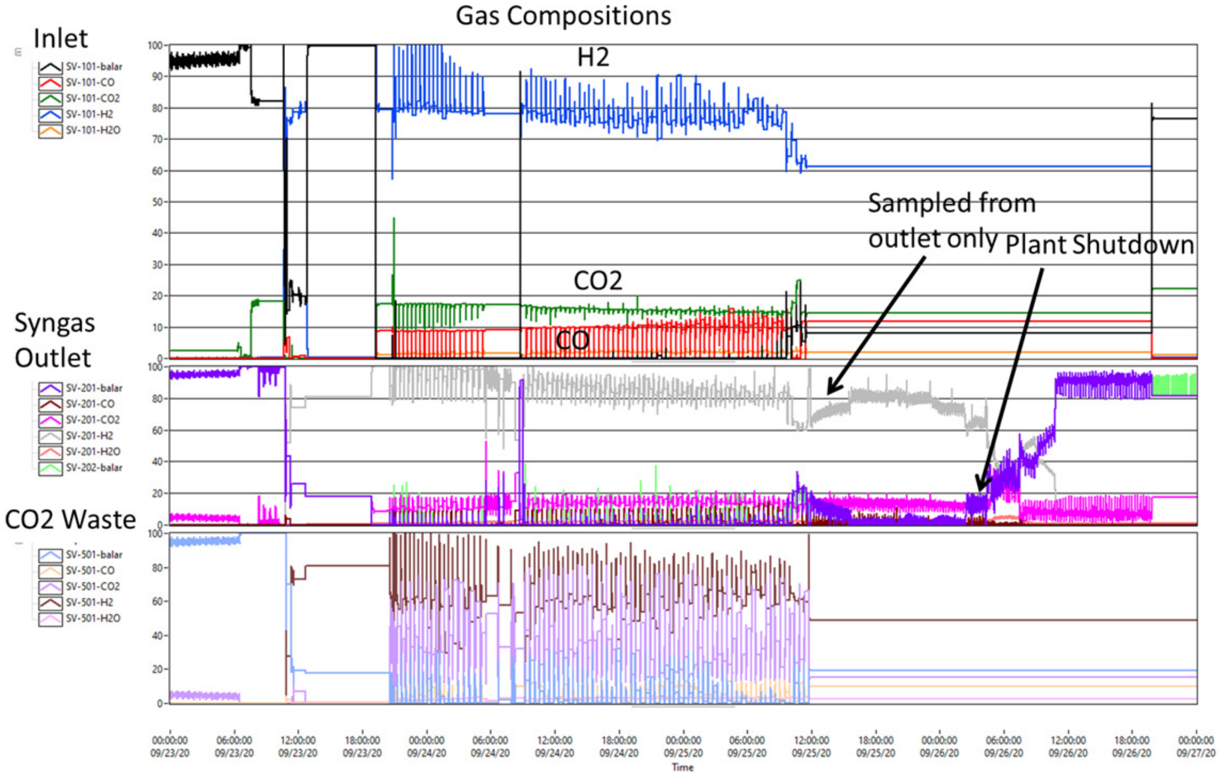


Figure 66. Campaign # 2: Gas compositions observed during the syngas testing.

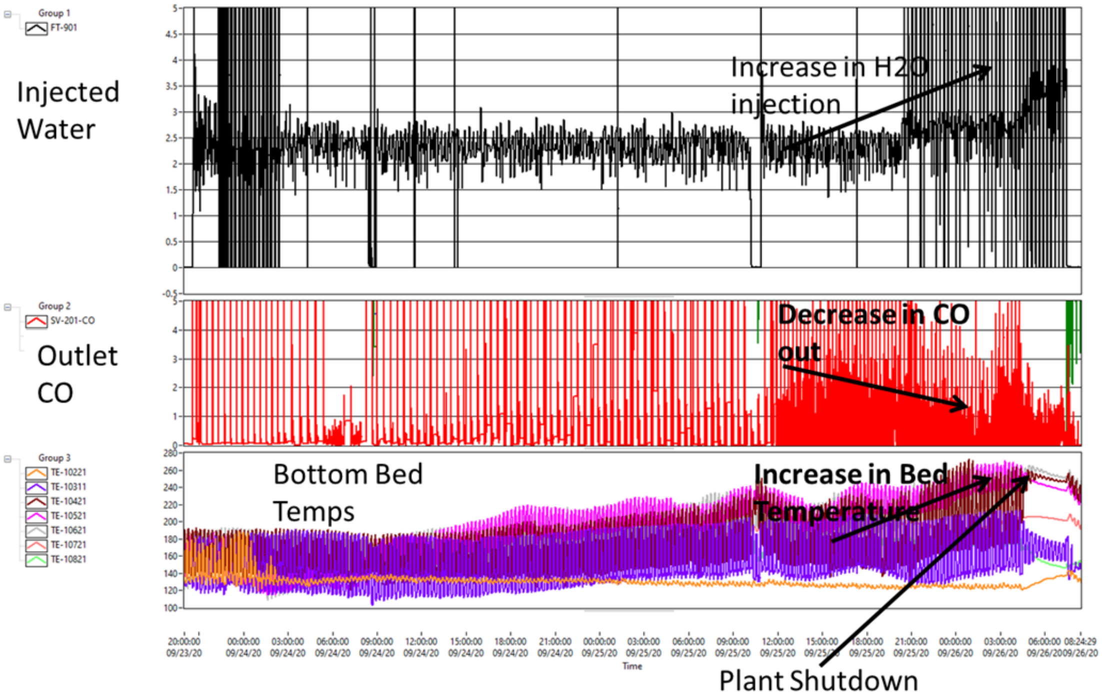


Figure 67. Campaign # 2: Bed temperatures and water injection rates during the syngas testing.

We were able to achieve 90-95% CO conversion within the bed at low steam to CO ratios (~1). We briefly increased the water injection amount by 25% and outlet CO dropped from 2% to sub 1% while the bed temperatures in the bottom (catalyst zone) rose by nearly 60C (Figure 67). This happened right before the plant shutdown, otherwise the plan was to keep increasing the injected water amount to see its effects on bed temperatures as well as get > 97% CO conversion.

Praxair's sump pump broke after we had returned to Colorado. We were able to restart the system remotely. However, we then observed increases in pressure drop and issues with flowing out of the system. With the help of one of Praxair's engineers, we observed that a large amount of sorbent was escaping the beds making its way downstream and plugging the lines and filters (Figure 68).

Figure 68. Carbon dust accumulation downstream.

Many attempts were made to clean the system out in which we then ran on N_2 and CO_2 to see if the problem would go away. Unfortunately, it continued to be a problem. We concluded that more than one of the bed's retention screens must have been breached, allowing sorbent to escape. It was during this time, the state of New York heavily restricted travel from other states including Colorado, which require us to do 2-week quarantine before we get on-site and we determined there was not enough time to make a trip to fix the issues. Also, Praxair required the space that our system was using to start up a new project they had for their OTM. It was determined that the system needed to be decommissioned and shipped back to Colorado. In early December, 2020 the system was disconnected, shrink wrapped and shipped back to Colorado where it resides on TDA's property.

CFD Model Validation with Field Test Data:
With the calibrated CFD model setup from 2018 as the basis of simulation, the following changes in system operating conditions were modeled to approximate that of the operating test at a Praxair facility in September 2020 (Figure 69). These conditions include:

Inlet syngas had the average properties outlined in Table 9 below, during the 4.0 minute adsorption step. As compared to the calibration scenario (appendix), this case has a greater syngas flow rate (~1.5X) and greater concentration of CO (~2.0X), thus the maximum spray cooling necessary to absorb the WGS heat release is greater, at approximately 1.15 kW (~2.0 kg/h of cooling water).

Water injection is performed at the lowest injector only (middle and upper injectors are disabled), timed with the adsorption step only. Using a *MW085* spray nozzle, the BETE MicroWhirl®, water is injected at 867 psig which per the nozzle's specification sheet corresponds to approximately 5.6 kg/h with a cone-shaped fog. Presumably this spray is in excess of the aforementioned estimated cooling need to provide excess water to drive the WGS reaction.

Regeneration steam, while not used in this current analysis focusing on the adsorption step only, drives the sorbent regeneration step for 3.5 minutes each cycle with 100 SLPM of 50 psig steam at an inlet temperature of 110°C.

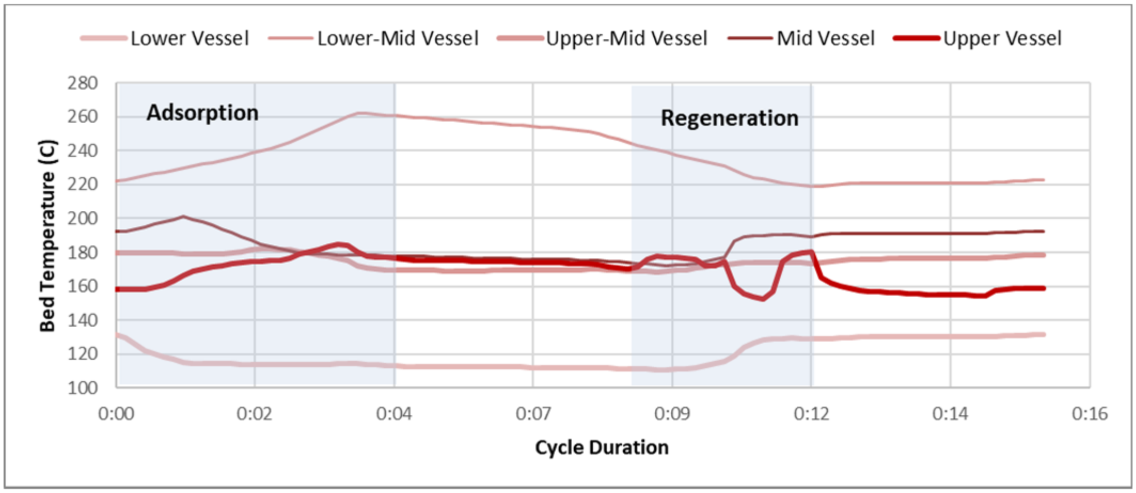


Figure 69. Chart of Bed Temperatures from Field Dataset for Full Cycle (9/20)

Table 9. Boundary Conditions from Current Model.

Case	Syngas Flow Rate (SLPM)	CO2 %	CO %	H2O %	H2 %	CH4 %	Inlet Temp. (°C)	Bed Pressure (PSIG)
Praxair (9/20)	415 SLPM	16.6	9.3	1.0	73.1	0	130	324

Using the calibrated model and these operating conditions, GTI ran a series of steady state simulations to investigate the “worst case” scenario as with the 2018 update. The sequence of simulations began with a baseline step (no spray cooling or WGS), then added WGS reactions and gradually increased the spray mass flow rate to ensure numerical stability due to issues noted previously, including backflow and disproportionately high sorption rates at the inlet section. Figure 70 shows the comparison of the

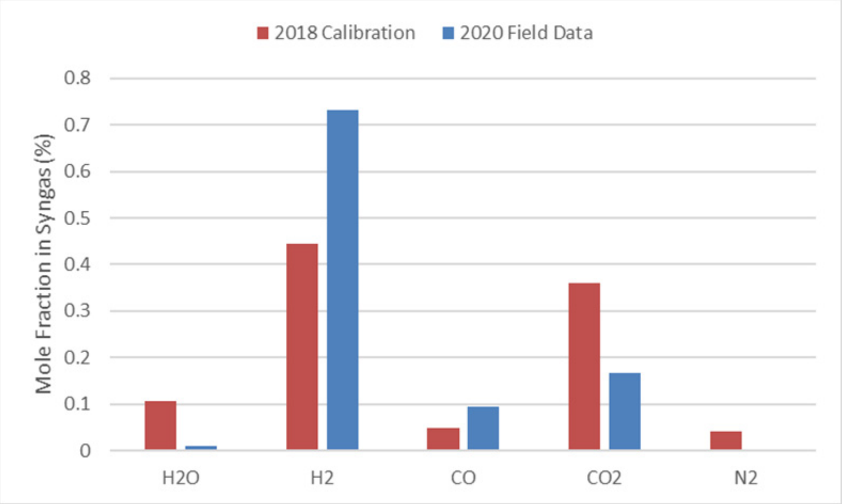


Figure 70. Comparing Inlet Syngas Composition.

synthesis gas composition used in our original CFD model calibration from tests at TDA in 2018 and the Praxair Tests in the Second Test Campaign in 2020.

The resulting sorbed CO_2 in the sorbent sections is shown in Figure 72, for the case with and without active spray cooling at the lowest level per above. Here, we can see that the impact of spraying from zero (left), to low spray (~50% of target), to high spray case (target flow) is not as significant as one would expect, the net volume of sorbed CO_2 in these cases at the peak case does not change substantially. These steady state solutions represent the peak sorption levels, primarily a function of bed temperatures for a given inlet concentration, and do not represent expected sorption levels for a cycling, multi-bed system. This is due to the fact the PraxairField tests during the second campaign was run with longer cycle times.

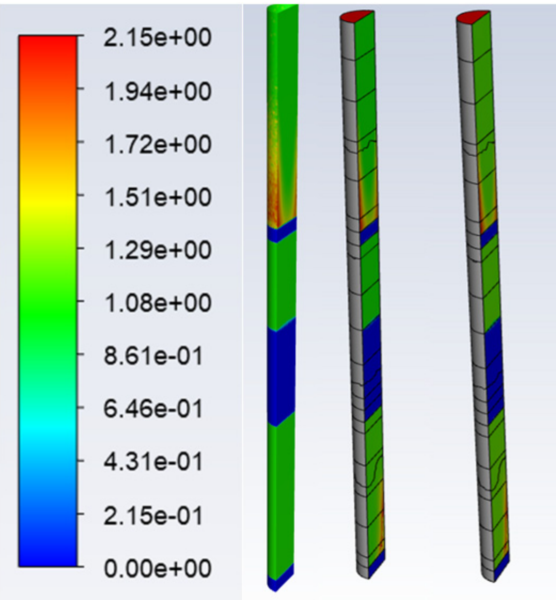


Figure 72. Steady State Sorbed CO_2 without (Left) and with Spray Cooling in Low (Mid) and High Case (Right) [mol CO_2/kg sorbent].

Figure 71 highlights the visualization of the spray which per the field dataset and resulting assumptions operates with a significantly higher throughput as compared to the original calibration dataset by a factor of ~20X. This significantly higher throughput, longer/narrower orifice, and higher source pressure pushes the limits of the embedded *plain orifice atomizer* model within the discrete phase particle modeling module. This modeling approach, originally calibrated in the aforementioned 2018 study, focused on calibrating the three spray nozzles to the expected level of cooling and WGS reaction heat absorption. This approach outlined in a prior update included an investigation of sensitivity of the *plain orifice atomizer* model parameters, including C_A, L/D of the nozzle, total flow rate, and investigating the impact of gravity vs. syngas flow rate. While the range of C_A and the modeling of gravity is fed forward to this case here, the boundary conditions impacting L/D and total flow rate are much higher than from the calibration dataset, ~8X and ~20X higher respectively. As noted, this extends beyond the structured limitations of the *plain orifice atomizer* due to the dynamic of droplet size distribution, cavitation, and other factors. Therefore, future modeling efforts should address the limitations of the orfice assumptions in the current model. There are 10 alternative models possible within the CFD code in addition to customized approaches (as were applied to CO_2 sorption).

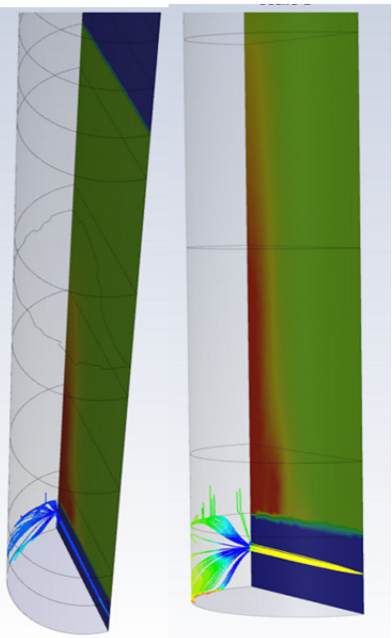


Figure 71. Spray Shown in Lower Reactor for Low and High Cases (Left/Right).

5.17 Tasks 7, 13, and 18. Long-Term durability Tests


Figure 73. Picture of the test apparatus.

Test System: We used an existing flow apparatus to evaluate the performance of the materials under representative conditions (Figure 73). The materials were exposed to a mixture of H_2, CO, CO_2, H_2O, and N_2. Electronic mass flow controllers were used to introduce the gas streams of H_2, CO, CO_2, and N_2. H_2O was introduced into the system with a high-pressure liquid pump.

Prior to testing, these gases are heated to about 160°C and mixed before entering the reactor. The system pressure is controlled with a Badger pressure control valve located at the downstream of the bed. The feed gas mixture is either directed through the sorbent/catalyst bed or through a by-pass loop for the analysis of the feed gas. The system is further plumbed so that the material can be tested by adsorbing with the gases entering from the top of the reactor and regenerating with a counter-current flow, or with the both the adsorption and regeneration gases from the top down.

The gas stream exiting the module or by-pass loop was then directed NOVA analyzer to determine the CO_2, CO, CH_4 and H_2 levels. In later testing a California Analyzer was used instead for CO_2 and CO. Labview software was used to control the apparatus and provided us unattended operation capability, including tests overnight. Safety precautions were in place and in case of overheating, over pressurization, or hazardous gas leak, both hardware and software will automatically shutdown the system.

Material Cycling: Prior to testing the combined sorbent and catalyst bed, the sorbent itself was cycled over 1500 times in N_2 and CO_2. This testing was done in advance to develop the programing for the system. After this testing was completed, some of the sorbent was removed and replaced with the catalyst. Half the catalyst was placed at the top of the bed and the other half was mixed with the remaining sorbent in a layer underneath.

Once the combined material was loaded the initial cycles were done in N_2 and CO_2 (cycles 1-~500 in Figure 74). H_2, CO and H_2O were then added to the mixture (adsorb: 45-50% H_2, 30% CO_2, 7% H_2O, 2-4% CO and balance N_2, regen: 25% H_2O, and balance N_2) and the initial adsorptions were done at 300 psig and the regenerations at 50 psig. The bed temperature has been maintained at ~200° throughout the testing. (The adsorption temperature and regeneration profiles are given in Figure 75.). The CO_2 loadings are calculated using only the inlet CO_2, not adding in the CO_2 formed by the water gas shift reaction. Other minor changes made to the testing are show in the event log (Figure 77).

At cycle ~2000, we dropped the adsorption pressure to 150psig. At cycles 22,761 and 30,072 the pressure was again raised to 300 psig for periods of testing.

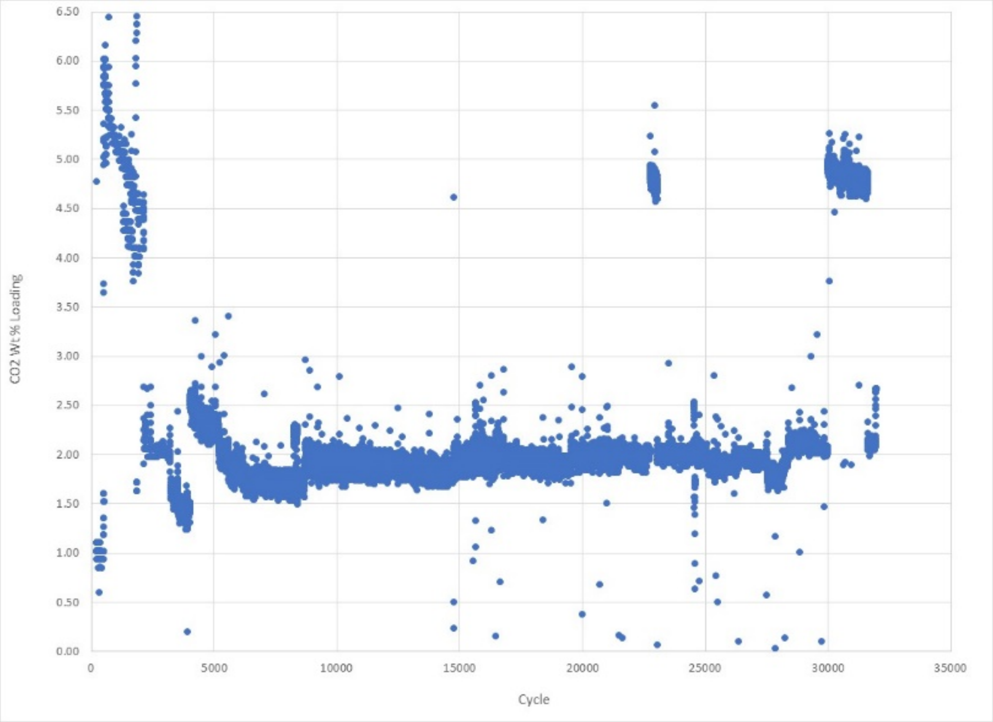


Figure 74. CO_2 loading in sorbent/catalyst cycling data.

Between cycles 25,363-26,350 we increased the CO inlet to 6% (lowering the CO_2 to maintain the carbon inlet) and increased the water (lowering the N_2 to maintain the total flow.) This didn't appear to harm the material, the performance constant when the CO was returned to the original inlet.

We also looked at the influence of water level in the regeneration gas increasing the inlet from the 33% H_2O used in the majority of the testing to 50% between cycles 27,516 and 28,373. The bed's performance remained largely stable maintaining a CO_2 working capacity of 2% wt. CO_2 over the 31,600 cycles that were carried out in total.

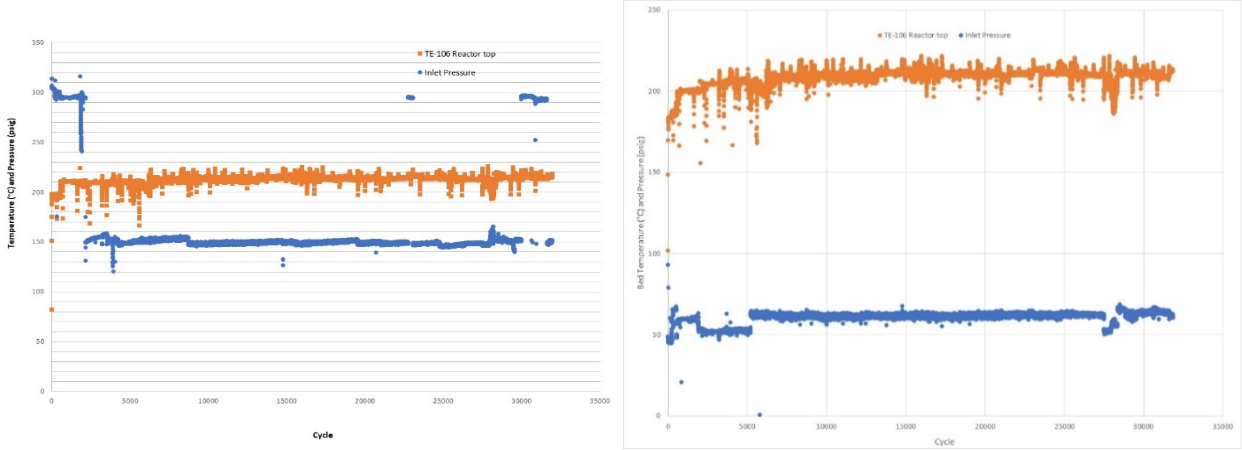


Figure 75. Adsorption (left) and regeneration (right) temperature and pressure.

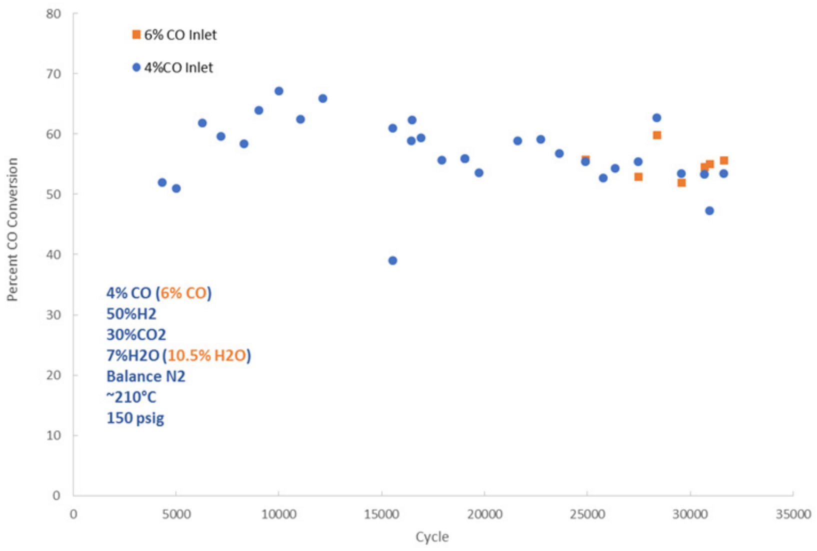
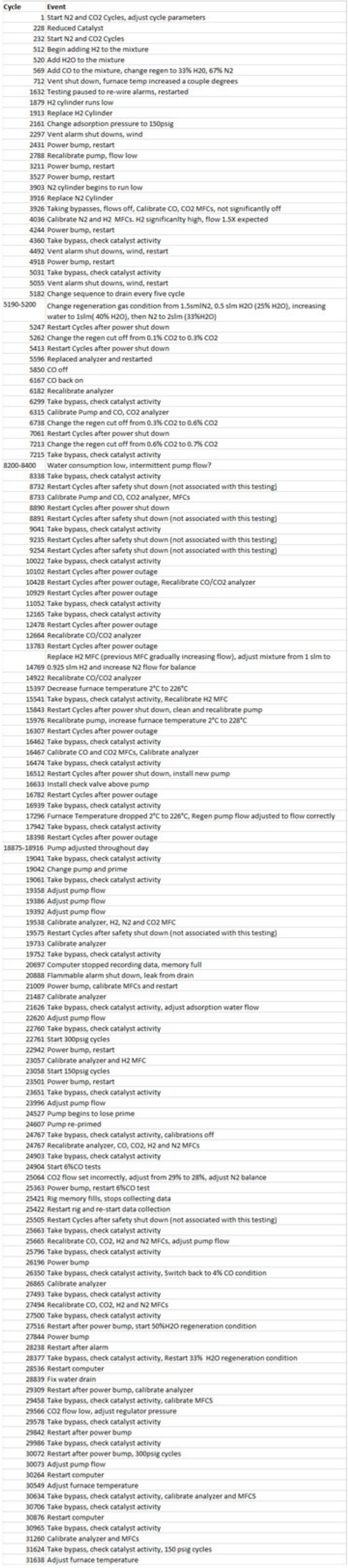


Figure 76. WGS catalyst activity during the long-term durability test of integrated WGS catalyst/CO_2 sorbent bed in bench-scale.

We also carried out tests intermittently to verify that the WGS catalyst maintained its activity by carrying out extended cycle tests that had a 15 min long adsorption step. In these tests we verified that the CO conversion remained the same between 50-60% after CO_2 breakthrough as we cycled the sorbent. In these tests the sorbent bed was saturated with CO_2 and the steady state conversion after the 15 min is reported. Hence, the CO conversion was much lower than those observed during the shorter cycles. In the shorted cycles during the long-term durability tests where we operate the sorbent bed to CO2 breakthrough, the CO_2 sorbent shifts the WGS reaction equilibrium thereby allowing us to achieve CO conversion in excess of 95%. Figure 76 shows the CO conversion with a simulated syngas composition of 4% CO, 50% H_2, 30% CO_2, 7% H_2) in balance N_2 at 210°C and 150 psig. The data shown in square symbols were those extended cycles where we had 6% CO and 10.5% H_2O in the simulated syngas stream.



Cycle	Event
1	Start N2 and CO2 Cycles, adjust cycle parameters
228	Reduced Catalyst
232	Start N2 and CO2 Cycles
512	Begin adding H2 to the mixture
520	Add H2O to the mixture
569	Add CO to the mixture, change regen to 33% H20, 67% N2
712	Vent shut down, furnace temp increased a couple degrees
1632	Testing paused to re-wire alarms, restarted
1879	H2 cylinder runs low
1913	Replace H2 Cylinder
2161	Change adsorption pressure to 150psig
2297	Vent alarm shut downs, wind
2431	Power bump, restart
2788	Recalibrate pump, flow low
3211	Power bump, restart
3527	Power bump, restart
3903	N2 cylinder begins to run low
3916	Replace N2 Cylinder
3926	Taking bypasses, flows off, Calibrate CO, CO2 MFCs, not significantly off
4036	Calibrate N2 and H2 MFCs. H2 significanlty high, flow 1.5X expected
4244	Power bump, restart
4360	Take bypass, check catalyst activity
4492	Vent alarm shut downs, wind, restart
4918	Power bump, restart
5031	Take bypass, check catalyst activity
5055	Vent alarm shut downs, wind, restart
5182	Change sequence to drain every five cycle
5190-5200	Change regeneration gas condition from 1.5smlN2, 0.5 slm H2O (25% H2O), increasing water to 1slm(40% H2O), then N2 to 2slm (33%H2O)
5247	Restart Cycles after power shut down
5262	Change the regen cut off from 0.1% CO2 to 0.3% CO2
5413	Restart Cycles after power shut down
5596	Replaced analyzer and restarted
5850	CO off
6167	CO back on
6182	Recalibrate analyzer
6299	Take bypass, check catalyst activity
6315	Calibrate Pump and CO, CO2 analyzer
6738	Change the regen cut off from 0.3% CO2 to 0.6% CO2
7061	Restart Cycles after power shut down
7213	Change the regen cut off from 0.6% CO2 to 0.7% CO2
7215	Take bypass, check catalyst activity
8200-8400	Water consumption low, intermittent pump flow?
8338	Take bypass, check catalyst activity
8732	Restart Cycles after safety shut down (not associated with this testing)
8733	Calibrate Pump and CO, CO2 analyzer, MFCs
8890	Restart Cycles after power shut down
8891	Restart Cycles after safety shut down (not associated with this testing)
9041	Take bypass, check catalyst activity
9235	Restart Cycles after safety shut down (not associated with this testing)
9254	Restart Cycles after safety shut down (not associated with this testing)
10022	Take bypass, check catalyst activity
10102	Restart Cycles after power outage
10428	Restart Cycles after power outage, Recalibrate CO/CO2 analyzer
10929	Restart Cycles after power outage
11052	Take bypass, check catalyst activity
12165	Take bypass, check catalyst activity
12478	Restart Cycles after power outage
12664	Recalibrate CO/CO2 analyzer
13783	Restart Cycles after power outage
14769	Replace H2 MFC (previous MFC gradually increasing flow), adjust mixture from 1 slm to 0.925 slm H2 and increase N2 flow for balance
14922	Recalibrate CO/CO2 analyzer
15397	Decrease furnace temperature 2°C to 226°C
15541	Take bypass, check catalyst activity, Recalibrate H2 MFC
15843	Restart Cycles after power shut down, clean and recalibrate pump
15976	Recalibrate pump, increase furnace temperature 2°C to 228°C
16307	Restart Cycles after power outage
16462	Take bypass, check catalyst activity
16467	Calibrate CO and CO2 MFCs, Calibrate analyzer
16474	Take bypass, check catalyst activity
16512	Restart Cycles after power shut down, install new pump
16633	Install check valve above pump
16782	Restart Cycles after power outage
16939	Take bypass, check catalyst activity
17296	Furnace Temperature dropped 2°C to 226°C, Regen pump flow adjusted to flow correctly
17942	Take bypass, check catalyst activity
18398	Restart Cycles after power outage
18875-18916	Pump adjusted throughout day
19041	Take bypass, check catalyst activity
19042	Change pump and prime
19061	Take bypass, check catalyst activity
19358	Adjust pump flow
19386	Adjust pump flow
19392	Adjust pump flow
19538	Calibrate analyzer, H2, N2 and CO2 MFC
19575	Restart Cycles after safety shut down (not associated with this testing)
19733	Calibrate analyzer
19752	Take bypass, check catalyst activity
20697	Computer stopped recording data, memory full
20888	Flammable alarm shut down, leak from drain
21009	Power bump, calibrate MFCs and restart
21487	Calibrate analyzer
21626	Take bypass, check catalyst activity, adjust adsorption water flow
22620	Adjust pump flow
22760	Take bypass, check catalyst activity
22761	Start 300psig cycles
22942	Power bump, restart
23057	Calibrate analyzer and H2 MFC
23058	Start 150psig cycles
23501	Power bump, restart
23651	Take bypass, check catalyst activity
23996	Adjust pump flow
24527	Pump begins to lose prime
24607	Pump re-primed
24767	Take bypass, check catalyst activity, calibrations off
24767	Recalibrate analyzer, CO, CO2, H2 and N2 MFCs
24903	Take bypass, check catalyst activity
24904	Start 6%CO tests
25064	CO2 flow set incorrectly, adjust from 29% to 28%, adjust N2 balance
25363	Power bump, restart 6%CO test
25421	Rig memory fills, stops collecting data
25422	Restart rig and re-start data collection
25505	Restart Cycles after safety shut down (not associated with this testing)
25663	Take bypass, check catalyst activity
25665	Recalibrate CO, CO2, H2 and N2 MFCs, adjust pump flow
25796	Take bypass, check catalyst activity
26196	Power bump
26350	Take bypass, check catalyst activity, Switch back to 4% CO condition
26865	Calibrate analyzer
27493	Take bypass, check catalyst activity
27494	Recalibrate CO, CO2, H2 and N2 MFCs
27500	Take bypass, check catalyst activity
27516	Restart after power bump, start 50%H2O regeneration condition
27844	Power bump
28238	Restart after alarm
28377	Take bypass, check catalyst activity, Restart 33% H2O regeneration condition
28536	Restart computer
28839	Fix water drain
29309	Restart after power bump, calibrate analyzer
29458	Take bypass, check catalyst activity, calibrate MFCS
29566	CO2 flow low, adjust regulator pressure
29578	Take bypass, check catalyst activity
29842	Restart after power bump
29986	Take bypass, check catalyst activity
30072	Restart after power bump, 300psig cycles
30073	Adjust pump flow
30264	Restart computer
30549	Adjust furnace temperature
30634	Take bypass, check catalyst activity, calibrate analyzer and MFCS
30706	Take bypass, check catalyst activity
30876	Restart computer
30965	Take bypass, check catalyst activity
31260	Calibrate analyzer and MFCs
31624	Take bypass, check catalyst activity, 150 psig cycles
31638	Adjust furnace temperature

Figure 77. Event log

5.18 Task 17. Process Design

UCI developed the Aspen Plus V9.0 models for the IGCC power plant and the F-T liquids coproduction case with the E-Gas gasifier for the cold gas and warm gas cleanup cases. They have utilized the performance of the advanced WGS + PSA reactor from the previous completed study (DE-FE-0012048) to start this current study. An analysis of the two F-T cases is showing that the degree of shifting required is very small, about 3% of the syngas is being shifted to provide suitable feed to the PSA unit (which produces H2 for the F-T liquids hydrocracking and hydrotreating operations) while the entire feed gas to the F-T synthesis unit is the unshifted gas. Due to the ability of the iron-based F-T catalyst to promote water gas shift in situ, the F-T reactor requires a relatively low H2/CO molar ratio of 1:1 to 1.1:1 (we have used a ratio of 1.05) while the raw syngas produced by the E-Gas gasifier has H_2/CO molar ratio 1.015. Thus, the advantage of the combined WGS+PSA unit has a minor effect on the overall plant performance in the case of FT liquid production.

However, we observed that TDA's integrated WGS/high temperature PSA (pressure-swing adsorption)-based Warm Gas Clean-up Technology can make a substantial improvement in the IGCC plant's thermal performance when the design objective is to achieve near zero emissions, including greater than 90% carbon capture. The increase in net plant efficiency for E-Gas^{TM} is 3.5% point compared to an IGCC power plant using E-Gas technology with cold gas capture. So, in this project UCI updated process models in AspenPlus® for the Integrated WGS precombustion carbon capture process integrated to IGCC power plant.

In this project, as part of process design and optimization, we also worked with Indigo Power Systems (IPS) to optimize the concepts and input for integration of the advanced gas turbines into the IGCC to maximize performance. These included increasing the fidelity of the gas turbine model and the conversion of the turbine in the analysis to an advanced Siemens F-class gas turbine, assessment of results (Siemens vs. GE gas turbine) and improvements to the performance and integration concepts.

5.18.1 Siemens F-class gas turbine in warm gas cleanup model

Integrating the Siemens F-class gas turbine, with TDA's warm gas cleanup system results in the gas turbines operating on the shaft power limit, and with expander gas flow reduced by 19%, due to a 30% reduction in gas turbine inlet mass flow. To achieve the target 16:1 pressure ratio, expander Stage 1 nozzle throat is reduced to increase the Stage 1 pressure ratio from 1.85:1 to 1.95:1. Rotor inlet temperature is reduced from the 1404°C in the cold gas cleanup case to 1378°C, due to the higher concentration of water and carbon dioxide in the expander gas. Gas turbine gross power is 490.05 MW as the gas turbines are on the shaft power limit of 500 MW, net plant power is 635.60 MW, and net plant HHV thermal efficiency is 35.90%. The higher performance vs. the GE 7F is due to increased technology level, including a higher firing temperature. Exhaust temperature is 639°C, which is nominally higher than optimal, and which will be reduced during the performance improvement investigation via increased compressor pressure ratio.

5.18.2 Performance improvement and integration concepts

Syngas pressure requirements

The simulation results for the revised syngas delivery pressure requirements, in which the nitrogen delivery pressure to the syngas mixer was reduced from 32.89 bara to 25.57 bara, yielded performance gains of 1.28 MW in net plant output (to 636.88 MW) and 0.08% points in net plant HHV thermal efficiency (to 35.98%), both due to reduced nitrogen compressor load.

Syngas dilution requirements and gas turbine air integration

Incorporating full air integration, excess nitrogen injection, and extraction air heat recovery into the previous case Siemens F-class IGCC with TDA's warm gas cleanup resulted in substantial performance improvement. Net plant output increased over 80 MW to 718.50 MW, and net plant HHC thermal efficiency increased 0.58% points to 36.56%. In addition to the performance improvement, the use of 100% air integration eliminates the air separation unit compressors and combines both ASU's into a single unit, both of which should yield reduced plant cost. The extraction air heat recovery configuration is shown in Figure 78 below. The gas turbines hardware is fully utilized, operating at the shaft power limit, and within 2% of the inlet flow limit.

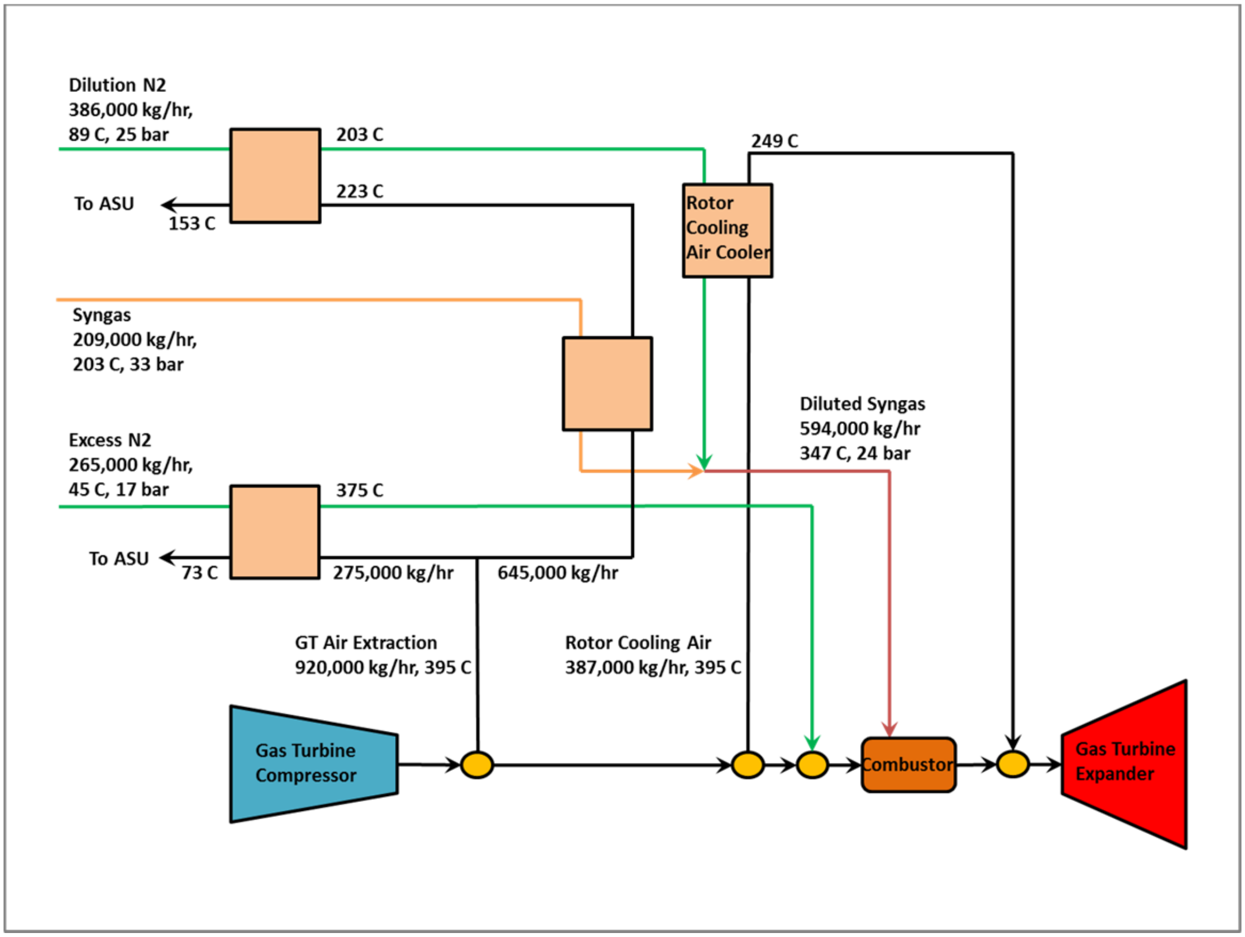


Figure 78. Air Integration - Extraction air heat recovery configuration.

Gas turbine pressure ratio

In the Siemens F-class turbine integrated with TDA's warm gas system, we updated syngas pressure requirements, and included full air integration, excess nitrogen injection, extraction air heat recovery, and with gas turbine pressure ratio increased to the 18.9:1 value of the original natural gas-fired Siemens F-class case. The simulation results indicate a loss in net plant output of 23.52 MW (to 694.97 MW) and a loss in net plant HHV thermal efficiency of 0.02% points (to 36.54%).

These results indicate that the optimal gas turbine pressure ratio is close to 16:1. In typical combined cycles, the optimal gas turbine pressure ratio occurs near that for a minimum approach to the first steam super-heater, but since we have air integration heat recovery, the effects of pressure ratio on that portion of the system cause the optimal pressure ratio to be lower. In particular, the increased pressure ratio caused additional unrecoverable heat loss in the extraction air heat recovery system.

Assessment of Results

The performance results are summarized in Table 10 below. The highest performance is achieved by Case A2 - Siemens F-class gas turbine with revised syngas pressure, full air integration, excess nitrogen injection, and extraction air heat recovery. This configuration yields advantages of 163.57 MW in net plant output and 1.96 percentage points in net plant thermal efficiency over the base Case A with GE 7F gas turbine and no air integration.

Table 10. Performance summary.

Case	Case Description	Pressure Ratio	RIT (°C)	EGT (°C)	Gas Turbine Gross Power (MW)	Net Plant Power (MW)	Net Plant HHV Thermal Efficiency (%)
A	GE 7F, Warm Gas Cleanup	16	1307	558	433.54	554.93	34.60
A1	Siemens SGT6-5000F, Warm Gas Cleanup	16	1378	639	490.05	635.60	35.90
A1'	Case A1 + Revised Syngas Pressure	16	1378	639	490.05	636.88	35.98
A2	**Case A1' + 100% Air Integration, Excess N2 Injection**	**16**	**1380**	**622**	**490.05**	**718.50**	**36.56**
A3	Case A2 with original natural gas-fired pressure ratio	18.9	1382	593	489.93	694.97	36.54

The performance 'pathway' from Case A to Case A2 is shown schematically in the performance tracking plot of Figure 79 below.

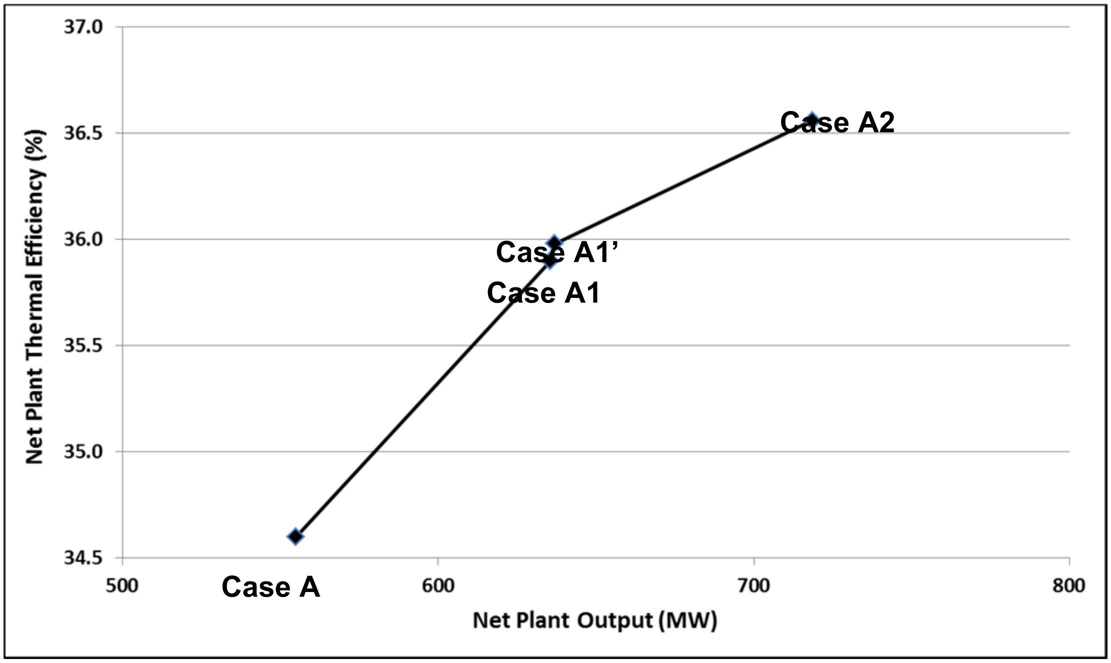


Figure 79. Performance tracking plot.

5.18.3 System Sizing and Costing

We completed the sizing and costing for the full scale combined WGS with CO_2 capture system. The results obtained for a design pressure of 39.4 bar and a design temperature of 260°C for a synthesis gas flow rate of 27,000 kmol/h containing 4.6% CO and 25.4% CO_2 achieving an overall CO conversion of 96+% is summarized in Table 11. The cost analysis was completed following DOE guidelines on a $2011 basis.

Table 11. Cost of the combined WGS with CO_2 capture system on $2011 basis.

Item/Description	Scale	$ 1,000							$116,117	
	Equipment Cost	Material Cost	Labor		Erected Cost	Eng Fee	Contingencies		Total Plant Cost	
			Direct	Indirect			Process	Project	$	$/kW
Vessels										
CO_2 Adsorption Vessels/Accumulators	$ 19,996	$ 20,536	$ 19,436		$ 59,968	$ 5,997	$ 11,994	$ 14,992	$ 92,951	
Vessel Internals	$ 2,565				$ 2,565	$ 257	$ 513	$ 641	$ 3,976	
Vessel Valves										
Vessel Valves	$ 2,363		$ 473		$ 2,836	$ 284	$ 567	$ 709	$ 2,363	
Train Isolation Valves	$ 159				$ 159	$ 16	$ 32	$ 40	$ 159	
Spares	$ 129				$ 129	$ 13	$ 26	$ 32	$ 129	
Pressure Relief	$ 211		$ 42		$ 253	$ 25	$ 51	$ 63	$ 211	
Compressor System										
Recycle Compressors	$ 5,018	$ 1,355	$ 1,480		$ 7,854	$ 785	$ 1,571	$ 1,963	$ 12,173	
Compressor Valves	$ 98				$ 98	$ 10	$ 20	$ 25	$ 153	
Water Knockout	$ 170	$ 175	$ 165		$ 510	$ 51	$ 102	$ 128	$ 791	
Heat Exchangers										
Shell and Tube	$ 75	$ 53	$ 46		$ 174	$ 17	$ 35	$ 43	$ 269	
Valves	$ 197				$ 197	$ 20	$ 39	$ 49	$ 305	
Water Injection System										
High Pressure Water Pumps	$ 447	$ 313	$ 303		$ 1,063	$ 106	$ 213	$ 266	$ 1,648	
Injection Valves	$ 159	$ 111	$ 32		$ 302	$ 30	$ 60	$ 75	$ 468	
Nozzles/Piping	$ 240	$ 48	$ 48		$ 336	$ 34	$ 67	$ 84	$ 521	

Figure 80 shows the distribution of the system cost between various subsystems. The vessel cost is the primary driver for the overall cost of the system. We also carried out sensitivity analysis varying the CO to CO_2 ratio and observed that very high CO to CO2 ratio's the cost of combined WGS system start increasing (Figure 81).

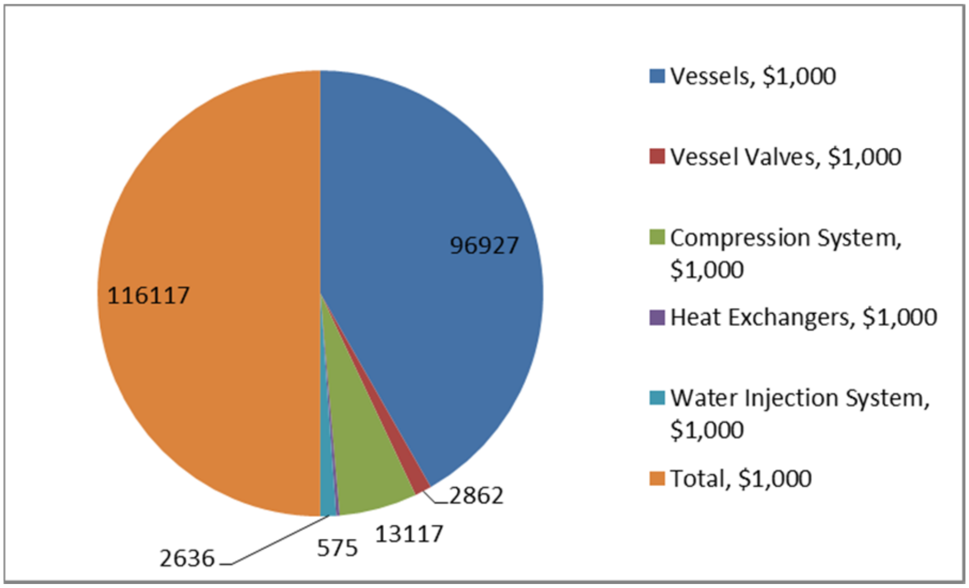


Figure 80. Cost distribution for various sub-system in the combined WGS with CO_2 capture (reported in $2011 basis on a $1,000 scale)

Preliminary TEA

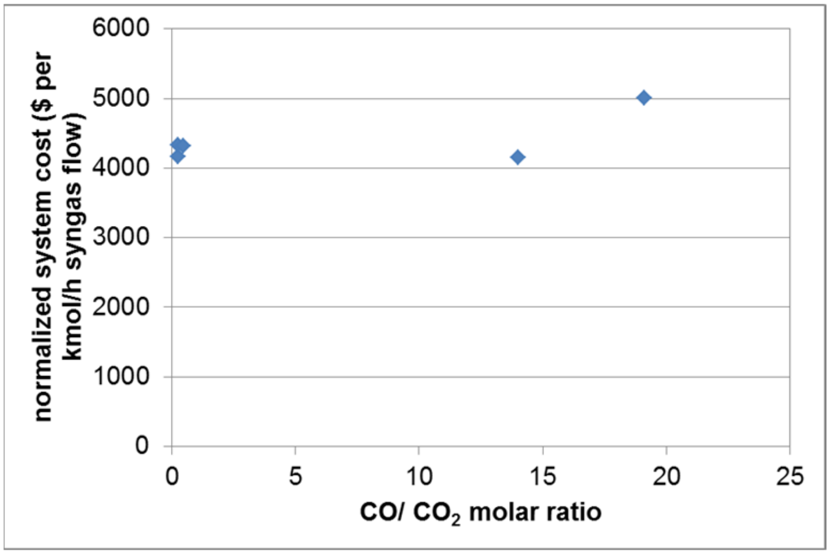


Figure 81. Normalized system cost per unit syngas flow as a function of CO/CO$_2$ molar ratio.

We completed the process design for the combined WGS based pre-combustion CO$_2$ capture system integrated to the IGCC power plant operating on coal based E-Gas^{TM} gasification system (Milestone 3-3). The system efficiency with preliminary cost numbers on a $2011 basis is provided in Table 12. For comparison the net plant efficiency and cost of capture numbers for the E-Gas^{TM} gasification system operating on Illinois No. 6 bituminous coal integrated with regular state-of-the-art cold gas and TDA's warm gas clean-up based CO$_2$ capture system (without integration with WGS) are provided. We see that the net plant efficiency was the highest for TDA's warm gas capture system when integrated with the last water gas shift stage at 34.7% vs 34.1% for the warm gas capture based system when it is not integrated with the WGS step. The increase in heat rate for the integrated WGS carbon capture system is about 12% over the cold gas cleanup based carbon system (Selexol^{TM}). The cost of carbon capture including TS&M is estimated to be $35.8 per tonne ($25.8 per tonne when excluding the TS&M costs) for the integrated WGS based capture system. This is lower than DOE target for transformational carbon capture technologies of $30 per tonne excluding TS&M costs.

Table 12. Comparison of different CO$_2$ capture system with E-GasTM based IGCC power plants. Rev. 2a - $2011 cost basis

Gasifier Type/Make	E-Gas		
Case	1	2	2* (WGS/CO$_2$)
CO$_2$ Capture Technology	Cold Gas Cleanup Selexol^{TM}	Warm Gas Cleanup TDA's CO$_2$ Sorbent	Warm Gas Cleanup TDA's CO$_2$ Sorbent
CO$_2$ Capture, %	90	90	90
Gross Power Generated, kW	710,789	670,056	693,542
Gas Turbine Power	464,000	425,605	427,980
Steam Turbine Power	246,789	244,450	265,562
Syngas Expander Power	-	-	-
Auxiliary Load, kW	194,473	124,138	138,741
Net Power, kW	516,316	545,917	554,801
Net Plant Efficiency, % HHV	31.0	34.1	34.7
Coal Feed Rate, kg/h	220,549	212,265	212,265
Raw Water Usage, GPM/MW	10.9	10.3	10.0
Total Plant Cost, $/kW	3,464	3,042	2,990
COE without CO$_2$ TS&M, $/MWh	136.8	120.5	118.8
COE with CO$_2$ TS&M, $/MWh	145.7	128.6	126.7
Cost of CO$_2$ Captured, $/tonne	**53.2**	**37.4**	**35.8**

5.19 Task 22. System Analysis

As part of the subcontract work, the Advanced Power and Energy Program (APEP) of the University of California, Irvine (UCI) has evaluated the combined water gas shift (WGS) reaction and high temperature pressure swing adsorption (PSA)-based CO_2 capture process being developed by TDA in IGCC and Fischer-Tropsch (F-T) liquids production plants. Process system simulations to assess the performance, cost and economics of this novel syngas decarbonization process for pre-combustion CO_2 capture technology applications ("Warm Gas Cleanup" cases) were made. The relative advantages in terms of performance and costs are compared to state-of-the-art conventional technology ("Cold Gas Cleanup" cases). Both E-Gas^{TM} type (will simply be identified as "E-Gas") and General Electric's GEP type (will simply be identified as "GEP") gasifier cases with a bituminous coal were evaluated in IGCC applications. Coproduction of synthetic fuels (and chemicals) is gaining significant attention due to the synergy between electricity generation and coproduction, especially with intermittent renewables supplying a larger fraction of power to the grid. Coproduction of F-T liquids was evaluated with the E-Gas gasifier, again with Cold Gas Cleanup and with Warm Gas Cleanup. Detailed Techno-economic analysis results are provided in Appendix A.

5.19.1 IGCC Cases

Comparing the two E-Gas cases, the heat rate with the Warm Gas Cleanup employing TDA's combined WGS and CO_2 PSA reactor is 10.3% lower, while at the same time the plant cost on a $/kW is reduced by about 12.7%, resulting in a decrease in the COE (with CO_2 TS&M costs included) by about 12.6%. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $26/tonne which is significantly lower than that for the Cold Gas Cleanup case at $43/tonne. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the SCPC (w/o CO_2 capture) for the Warm Gas Cleanup case is $47/tonne, again significantly lower than that for the Cold Gas Cleanup case at $62/tonne.

Next, comparing the two GEP cases, the heat rate with the Warm Gas Cleanup employing TDA's combined WGS and CO_2 PSA reactor is 8.5% lower, while at the same time the plant cost on a $/kW is reduced by about 6% resulting in a decrease in the COE (with CO_2 TS&M costs included) by about 7.7%. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $28/tonne which is significantly lower than that for the Cold Gas Cleanup case at $38/tonne. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the SCPC (w/o CO_2 capture) for the Warm Gas Cleanup case is $54/tonne, again significantly lower than that for the Cold Gas Cleanup case at $61/tonne. Improvement in efficiency over the corresponding Cold Gas Cleanup case is less pronounced when compared to the E-Gas cases because in the Warm Gas Cleanup E-Gas case, the CH_4 content was allowed to be higher.

These 1st year CO_2 capture costs compared to the supercritical pulverized coal (SCPC) power plant without CO_2 capture for the above Warm Gas Cleanup cases are much higher than when compared to the IGCC power plant without CO_2 capture. Note however, that comparison to the SCPC power plant may not be fair since this comparison does not account for the other environmental benefits that the IGCC power plant offers over the SCPC.

5.19.2 Fischer-Tropsch Cases

Both the Cold Gas Cleanup and Warm Gas Cleanup cases are designed for the same coal feed rate of 19,053 tonne/D (as received basis) consistent with the reference case summarized in DOE/NETL-2011/1477 which results in the production of 1,475 tonne/D naphtha and 3,632 tonne/D diesel in the Cold Gas Cleanup case, and 1,509 tonne/D naphtha and 3,601 tonne/D diesel in the Warm Gas Cleanup case. With the three GE 6B type gas turbine based combined cycles, the amount of excess power generated is 140 MW in the Cold Gas Cleanup case and as much as 253 MW in the Warm gas Cleanup case due to its higher efficiency. The majority of the power generated in these plants is by the steam turbine. The export power was credited at \$59.59/MWh while generating the 1st year required sales price (RSP) for the naphtha and for the diesel using the commercial fuel structure with capital charge factor of 0.218. The total plant cost for the Warm Gas Cleanup case is slightly lower than that of the Cold Gas Cleanup case (by about 1%). However, due to the significantly higher export power of the Warm gas Cleanup case, the RSP of the products is reduced over the Cold Gas Cleanup case. The RSP with CO_2 TS&M included was calculated to be \$120/bbl for the naphtha and \$172/bbl for the diesel in the case of Cold Gas Cleanup, and \$115/bbl for the naphtha and \$166/bbl for the diesel in the case of Warm Gas Cleanup, a decrease of more than 3% for each of these coproducts.

Appendix A

Final Techno-economic Analysis

TDA's Integrated WGS precombustion carbon capture Technology

FINAL REPORT SUBMITTED TO TDA RESEARCH, Inc

Department of Energy Contract No. DE-FE-0023684

Integrated Water-Gas-Shift Pre-combustion Carbon Capture Process

Prepared By

Advanced Power and Energy Program

University of California, Irvine

October 2021

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Table of Contents

1 Executive Summary

As part of the subcontract work, the Advanced Power and Energy Program (APEP) of the University of California, Irvine (UCI) has evaluated the combined water gas shift (WGS) reaction and high temperature pressure swing adsorption (PSA)-based CO_2 capture process being developed by TDA in IGCC and Fischer-Tropsch (F-T) liquids production plants. Process system simulations to assess the performance, cost and economics of this novel syngas decarbonization process for pre-combustion CO_2 capture technology applications ("Warm Gas Cleanup" cases) were made. The relative advantages in terms of performance and costs are compared to state-of-the-art conventional technology ("Cold Gas Cleanup" cases). Both E-Gas^{TM} type (will simply be identified as "E-Gas") and General Electric's GEP type (will simply be identified as "GEP") gasifier cases with a bituminous coal were evaluated in IGCC applications. Coproduction of synthetic fuels (and chemicals) is gaining significant attention due to the synergy between electricity generation and coproduction, especially with intermittent renewables supplying a larger fraction of power to the grid. Coproduction of F-T liquids was evaluated with the E-Gas gasifier, again with Cold Gas Cleanup and with Warm Gas Cleanup.

1.1 IGCC Cases

Comparing the two E-Gas cases, the heat rate with the Warm Gas Cleanup employing TDA's combined WGS and CO_2 PSA reactor is 10.3% lower, while at the same time the plant cost on a $/kW is reduced by about 12.7% resulting in a decrease in the COE (with CO_2 TS&M costs included) by about 12.6%. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $26/tonne which is significantly lower than that for the Cold Gas Cleanup case at $43/tonne. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the SCPC (w/o CO_2 capture) for the Warm Gas Cleanup case is $47/tonne, again significantly lower than that for the Cold Gas Cleanup case at $62/tonne.

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These 1st year CO_2 capture costs compared to the SCPC without CO_2 capture for the above Warm Gas Cleanup cases are much higher than when compared to the IGCC without CO_2 capture. Note however, that comparison to the SCPC may not be fair since this comparison does not account for the other environmental benefits that the IGCC offers over the SCPC.

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Both the Cold Gas Cleanup and Warm Gas Cleanup cases are designed for the same coal feed rate of 19,053 tonne/D (as received basis) consistent with the reference case summarized in DOE/NETL-2011/1477 which results in the production of 1,475 tonne/D naphtha and 3,632 tonne/D diesel in the Cold Gas Cleanup case, and 1,509 tonne/D naphtha and 3,601 tonne/D diesel in the Warm Gas Cleanup case. With the three GE 6B type gas turbine based combined cycles, the amount of excess power generated is

140 MW in the Cold Gas Cleanup case and as much as 253 MW in the Warm gas Cleanup case due to its higher efficiency. Majority of the power generated in these plants is by the steam turbine. The export power was credited at \$59.59/MWh while generating the 1st year required sales price (RSP) for the naphtha and for the diesel using the commercial fuel structure with capital charge factor of 0.218. The total plant cost for the Warm Gas Cleanup case is slightly lower than that of the Cold Gas Cleanup case (by about 1%). However, due to the significantly higher export power of the Warm gas Cleanup case, the RSP of the products is reduced over the Cold Gas Cleanup case. The RSP with CO_2 TS&M included was calculated to be \$120/bbl for the naphtha and \$172/bbl for the diesel in the case of Cold Gas Cleanup, and \$115/bbl for the naphtha and \$166/bbl for the diesel in the case of Warm Gas Cleanup, a decrease of more than 3% for each of these coproducts.

2 Introduction

As part of the subcontract work, the Advanced Power and Energy Program (APEP) of the University of California, Irvine (UCI) has evaluated the combined water gas shift (WGS) reaction and high temperature pressure swing adsorption (PSA)-based CO_2 capture process being developed by TDA in IGCC and Fischer-Tropsch (F-T) liquids production plants. Process system simulations to assess the performance, cost and economics of this novel syngas decarbonization process for pre-combustion CO_2 capture technology applications ("Warm Gas Cleanup" cases) were made. The relative advantages in terms of performance and costs are compared to state-of-the-art conventional technology ("Cold Gas Cleanup" cases). Both E-Gas™ type (will simply be identified as "E-Gas") and General Electric's GEP type (will simply be identified as "GEP") gasifier cases with a bituminous coal were evaluated. Coproduction of synthetic fuels and chemicals is gaining significant attention due to the synergy between electricity generation and coproduction, especially with intermittent renewables supplying a larger fraction of power to the grid.

3 Study Approach

The overall plant analysis is performed in the context of a stand-alone gasification plant and the simulations are developed within the framework of Aspen Plus®. The plant simulation models developed by APEP in previous studies conducted for the DOE/NETL are modified as required. All the IGCC cases utilizing the TDA technology include the upstream sour WGS reactor followed by warm gas desulfurization before the syngas enters the 2nd shift reactor consisting of the combined WGS/CO_2 capture reactor since TDA's testing has been primarily based on this configuration. Furthermore, a previous study conducted also under subcontract to TDA had shown that when deleting the 1st (sour) shift reactor and employing only the combined WGS/PSA reactor, the heat rate increased because more water (liquid) had to be injected into the combined WGS/PSA reactor. Inclusion of the 1st reactor (an adiabatic reactor) into the design allows the preheat of the feed gas to the warm gas desulfurization process without requiring an expensive feed/effluent interchanger with gas on both sides.

3.1 Process Design Basis and Methodology

Consistency is maintained between the cases developed under this study utilizing the TDA's combined WGS reaction and high temperature PSA-based CO_2 capture process (**Warm Gas Cleanup cases**) with the plants with CO_2 capture utilizing current state-of-the-art syngas cleanup and CO_2 capture technology (**Cold Gas Cleanup cases**). Furthermore, the Cold Gas Cleanup cases are modeled such that consistency is maintained as much as possible with the corresponding cases in the following DOE NETL study reports while the economic analysis is revised to June 2011 basis.

- *Cost and Performance Baseline for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity*, Revision 2a, September 2013, DOE/NETL-2010/1397.
- *Cost and Performance Baseline for Fossil Energy Plants, Volume 3a: Low Rank Coal to Electricity: IGCC Cases*, November 2010, DOE/NETL- 2010/1399.
- *Baseline Analysis of Crude Methanol Production from Coal and Natural Gas*, Revised October 15, 2014, DOE/NETL-341/101514.
- *Cost and Performance Baseline for Fossil Energy Plants, Volume 4: Coal-to-Liquids via Fischer-Tropsch Synthesis*, October 15, 2014, DOE/NETL-2011/1477.

Sizing of the reactor vessel and its costs for the combined WGS reaction and CO_2 PSA were developed by TDA along with the catalyst and adsorbent loadings.

All electricity only cases separate out 90% of the gaseous carbon compounds present in the syngas. The F-T liquids cases capture 91% CO_2 capture which in these cases is being defined as:

CO_2 capture, % = $[1- (C_{OUT} - C_{INAIR})/(C_{INFEED} * X_c - C_{SYNPROD})]*100$
where
$C_{OUT} = C_{HRSG} + C_{DRYER}$
C_{HRSG} = moles CO_2 in the HRSG stack
C_{DRYER} = moles CO_2 in the coal dryer stack
C_{INAIR} = moles CO_2 in gas turbine suction air
C_{INFEED} = moles Carbon in total coal feed
X_c = Fractional carbon conversion in gasifier
$C_{SYNPROD}$ = moles Carbon in coproduct

Site Conditions

The plant is designed for the following site specific conditions:

- International Standards Organization (ISO) ("mid-western") site ambient conditions for:
  - Elevation: Mean sea level
  - Dry bulb temperature: 15°C
  - Relative humidity: 60%
- Mechanical draft cooling towers with 11°C temperature rise for the cooling water are used. The above ambient conditions correspond to a wet bulb temperature of 10.8°C. A cooling water supply temperature of 15.56°C (60°F) is used which correspond to a reasonable approach temperature to the wet bulb temperature.

The coal characteristics are presented in Table 1. The site characteristics are assumed to be the same as in the previously referenced DOE/NETL study reports:

- Location: Greenfield
- Topography: Level
- Transportation: Rail
- Ash/Slag Disposal: Off Site
- Makeup Water: Municipal (50%) / Groundwater (50%)
- Access: Landlocked, having access by rail and highway

- CO_2 Storage: Compressed to 15.3 MPa, transported 80 kilometers and sequestered in a saline formation at a depth of 1,239 m.

It is assumed that the land area required for the cold gas and the warm gas cleanup cases is the same. As in the previously referenced DOE/NETL studies, 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.

Carbon Dioxide Product Specification

The specifications for the CO_2 product are based on the typical purity obtained by the Selexol™ cold gas cleanup process which was used in the previously referenced DOE/NETL reports without any further purification. The concentration of N_2 and Ar in the CO_2 stream coming off TDA's PSA unit is similar to what is typically obtained from a Selexol™ unit, i.e., without any further purification. This is done to be consistent with the DOE analysis referenced earlier. Table 2 summarizes the CO_2 specifications used for this analysis.

Case Matrix

Table 3 summarizes the various cases developed in this study.

Table 1. Coal Data

Coal	**Bituminous**	
Proximate Analysis	As Received, %	Dry Basis, %
Moisture	11.12	0
Ash	9.7	10.91
Volatile Matter	34.99	39.37
Fixed Carbon	44.19	49.72
Total	100	100
Ultimate Analysis		
Carbon	63.75	71.72
Hydrogen	4.50	5.06
Nitrogen	1.25	1.41
Sulfur	2.51	2.82
Chlorine	0.29	0.33
Ash	9.70	10.91
Moisture	11.12	0.00
Oxygen (by difference)	6.88	7.75
Total	100	100
Heating Value		
HHV, kJ/kg	27,113	30,506
HHV, Btu/lb	11,666	13,126
LHV, kJ/kg	26,151	29,544
LHV, Btu/lb	11,252	12,712
Trace Components		
Mercury, ppm		0.15

Table 2. CO_2 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_2O Concentration ppmv	< 150

Table 3. Case Matrix

Case	Gasifier Type	Gas Treating	Product(s)
1	E-Gas	Cold gas with Selexol	Electricity
2	E-Gas	Warm gas with TDA’s WGS + CO2 PSA	Electricity
3	GE	Cold gas with Selexol	Electricity
4	GE	Warm gas with TDA’s WGS + CO2 PSA	Electricity
5	E-Gas	Cold gas with Rectisol	F-T Liquids + Electricity
6	E-Gas	Warm gas with TDA’s WGS + CO2 PSA	F-T Liquids + Electricity

4 Process Descriptions: Electricity Only (Cases 1 through 4)

Each of the reference Cold Gas Cleanup cases (Cases 1 and 3) was first modeled in Aspen Plus® and the overall thermal performance of the plant was compared to the corresponding case of the DOE/NETL baseline study in order to validate the Aspen Plus® model developed for the entire IGCC system. Changes in the plant configuration were made where necessary. The Warm Gas Cleanup cases (Cases 2 and 4) were then modeled in Aspen Plus® while maximizing consistency with the corresponding Cold Gas Cleanup cases.

4.1 Cold Gas Cleanup Cases 1 and 3

The IGCC plants employing the cold gas cleanup and CO_2 capture technology consist of the following plant subsystems:

- Air Separation Unit (ASU)
- Coal Feed Preparation
- Gasification (similar to E-Gas™ or GEP gasifier)
- High Temperature Syngas Cooling and Scrubbing
- Two Stage Sour Shifting and Heat Recovery
- Cold Gas Syngas Desulfurization and Decarbonization or acid gas removal (AGR) using a two-stage Selexol™ process
- Claus Sulfur Recovery and Tail Gas Hydrogenation (followed by recycle to the acid gas removal unit)
- CO_2 Dehydration and Compression
- Gas Turbines (similar to GE FA class technology)
- Heat Recovery Steam Generators (HRSGs)
- Reheat Steam Turbine

The plants also have the necessary utilities (e.g. cooling water supply, make-up water treatment, plant and instrument air) to support the process units. Detailed process descriptions of these cases may be found in the previously referenced DOE/NETL reports.

4.2 Warm Gas Cleanup Cases 2 and 4

The IGCC plants employing the warm gas cleanup and CO_2 capture technology consist of the following plant subsystems:

- ASU
- Coal Feed Preparation
- Gasification (similar to E-Gas™ or GEP gasifier)
- High Temperature Syngas Cooling and Scrubbing
- Warm Gas Cleanup (similar to RTI's process including H_2SO_4 Unit)
- Heat Recovery and Combined Shifting and Regenerable Sorbent CO_2 Capture
- CO_2 Purification and Compression
- Gas Turbines (similar to GE FA class technology)
- HRSGs
- Reheat Steam Turbine

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

The overall configurations of the warm gas cleanup IGCC plants with the combined reactor for WGS reaction and CO_2 PSA are shown in Figure 1 and Figure 2 for the E-Gas cases and Figure 3 and Figure 4 for the GEP cases. The corresponding stream data are presented in Table 4 and Table 5. Plant subsystems that are different from the corresponding Cold Gas Cleanup cases are described in the following.

Scrubbed gas is preheated to a temperature of 215°C in a feed/effluent exchanger and supplied to a sour shift reactor (in the case of the E-Gas gasifier case, a fraction of the raw syngas exiting the scrubber is compressed and recycled back to the gasifier system as raw syngas quench gas). Effluent from the reactor is then fed 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 H_2SO_4 from the SO_2 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 H_2SO_4 unit. The on-site ASU provides the small amount of O_2 as required by the H_2SO_4 unit in addition to supplying O_2 to the gasifier and the catalytic combustor used for CO_2 purification (to combust the residuals amounts of H_2, CO and CH_4). The hot syngas leaving the desulfurizer is cooled in an intermediate (IP) steam generator followed by the feed/effluent exchanger where the sour shift reactor feed gas is preheated. The partially shifted desulfurized syngas is further cooled in a medium pressure (MP) steam generator to a temperature of 210°C. Effluent from this exchanger is treated in TDA's expendable warm gas Hg removal system. The design uses lead-lag beds with 3 month change out. Some of the NH_3 and HCN are also removed by this process.

The treated syngas is then combined with recycle gas from TDA's combined WGS/PSA capture reactor for decarbonizing the syngas before it is combusted in the gas turbines. In the GEP case, a small fraction of the syngas bypasses the combined WGS/PSA capture unit to limit the overall carbon capture to 90%, the per-pass capture being significantly higher (about 98.1% of the CO_2 entering with the syngas is separated). The decarbonized syngas along with any bypassed syngas is sent directly to the gas turbine without requiring any humidification due to the large amount of steam introduced into the syngas in the TDA process. Regeneration is accomplished utilizing steam at a desorption pressure of about 10 barA. Two streams are regenerated, one consisting of "raw CO_2," a mixture of CO_2, steam and small amounts of residual syngas at a temperature of 190°C, and the other "recycle gas," with significant amounts of the combustibles (the other syngas components, mainly H_2) at a temperature of 235°C for recycle to the CO_2 separation unit. The raw CO_2 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 fed to a catalytic (noble metal) combustor along with O_2 from the ASU to oxidize the small amounts of combustibles present in the raw CO_2 stream. The effluent from this combustor after generating high pressure (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 dehydrated and further compressed in an intercooled compressor to the final plant battery limits pressure as specified in the design basis.

The decarbonized syngas leaving the CO_2 separation (adsorption) unit at a temperature of 203°C with its accompanying unreacted steam is supplied to the gas turbines along with pressurized N_2 from the ASU. However, the amount of N_2 added to the gas turbine 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 that uses a reheat steam cycle.

5 Process Descriptions: Fischer-Tropsch Liquids Coproduction (Cases 5 and 6)

The overall configurations of the cold gas cleanup and warm gas cleanup plants with the combined reactor for WGS reaction and CO_2 PSA are shown in Figure 5 and Figure 6. The combined reactor for WGS reaction and CO_2 PSA for Case 6 is shown in Figure 7. The corresponding stream data for Case 6 are presented in Table 6.

The plant configurations are similar to those of the previously described corresponding electricity only cases except that the coproducing plants in addition to containing the synthesis unit have:

- In addition to coal, purge gas from the F-T synthesis unit (to limit the build up of the lighter hydrocarbons within the synloop) is supplied to the gasifiers where these hydrocarbons are partially oxidized to form additional syngas.
- Rectisol unit for acid gas removal instead of Selexol™ in the Cold Gas Cleanup Case 1 in order to minimize the sulfur content of the syngas, sulfur containing compounds such as H_2S and COS being F-T synthesis catalyst poisons.
- Three GE 6B type gas turbines instead of two GE FA class type gas turbines to maximize coproduct production rate while generating enough power by the combined cycle to satisfy in-plant consumption.
- ASU's that provide a much lower fraction of pressurized N_2 for gas turbine injection than in the electricity only cases due to the lower gas turbine capacities.

Major differences existing in the configuration of the gas treatment and conditioning units are described in the following.

5.1 Cold Gas Cleanup Case 5

Majority of the scrubbed syngas is bypassed around the shift unit since the specified molar ratio of H_2 to CO of 1.05 in the feed to the first F-T synthesis reactor is already met. Note that the addition of purge gas from the F-T unit to the gasifier increases the H_2/CO ratio in the syngas to above 1.0 which would not be the case with just the bituminous coal feed. The fraction of the syngas shifted is based upon the H_2 demand of the hydrotreating and hydrocracking of the F-T liquids. The shifted and the bypassed streams are combined and fed to the low temperature gas cooling unit where the syngas is cooled in a series of heat exchangers and bulk of the mercury removed as in the corresponding electricity only case, and then fed to a Rectisol unit for desulfurization and decarbonization. A fraction of the treated syngas leaving the Rectisol unit is provided to a PSA unit to provide H_2 required by the F-T liquids processing and the remainder to the F-T synthesis unit.

F-T unit makeup syngas is preheated to 193°C and expanded in a turboexpander from a pressure of 33.6 bar to 23.5 bar as required by the synloop. The turboexpander is connected to the motor assisted synloop recycle compressor. The expanded gas is combined with the synloop recycle gas after the recycle gas is cooled in a series of heat exchangers and treated in an amine wash unit to remove CO_2 to satisfy the required Riblette rato $[(\text{FEED } H_2 - \text{FEED } CO_2)/(\text{FEED CO} + \text{FEED } CO_2)]$of 0.9837 at the reactor inlet. The combined stream is then preheated by a feed/effluent interchanger before being fed to a slurry reactor with Fe based catalyst particles suspending in an inert hydrocarbon liquid (a mineral oil). The mineral oil acts as a temperature moderator and a heat removal medium, transferring the heat of reaction from the catalyst surface via the liquid slurry to boiling water in an internal tubular heat exchanger. IP steam is generated from the heat. The major overall reactions occurring are: $(2n+1)\ H_2 + n\ CO = H\text{-}(CH_2\text{-})_n\text{-}H + n\ H_2O$ and $CO + H_2O = CO_2 + H_2$. The reactor effluent at 253°C is cooled against BFW, in the feed/effluent interchanger and then in a series of heat exchangers to condense out the liquids followed by preheating in a second interchanger before being fed into a second slurry reactor for additional conversion. The effluent from this second rector at 253°C is cooled against BFW, in the feed/effluent interchanger and then in a series of heat exchangers to condense out the liquids. The condensate collected after removing the decanted water is fed to a distillation column operating at 2 bar to remove the light ends, the bottoms from which are then fed to a vacuum column operating at 0.04 bar. The overhead condensate is fed to a hydrotreater to produce the naphtha coproduct while the bottoms are treated in a hydrocracker to produce the diesel coproduct. The overhead vapors from these operations are combined with the PSA tail gas and purge gas and then compressed before being recycled to the gasifier. A fraction of the purge gas is preheated to a temperature of 203ºC and supplied to the gas turbines in the combined cycle unit.

5.2 Warm Gas Cleanup Case 6

A major fraction of the scrubbed raw syngas is preheated to a temperature of 472°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 H_2SO_4 from the SO_2 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 H_2SO_4 unit. The on-site ASU provides the small amount of O_2 as required by the H_2SO_4 unit in addition to supplying O_2 to the gasifier and the catalytic combustor used for CO_2 purification (to combust the residuals amounts of H_2, CO and CH_4). The hot syngas leaving the desulfurizer is cooled in the feed/effluent exchanger. The remaining fraction of the scrubbed raw syngas is compressed and recycled back to the gasifier system as raw syngas quench gas. The desulfurized syngas is further cooled in a medium pressure (MP) steam generator to a temperature of 210°C. Effluent from this exchanger is treated in TDA's expendable warm gas Hg removal system. The design uses lead-lag beds with 3 month change out. Some of the NH_3 and HCN are also removed by this process.

Majority of the desulfurized syngas is bypassed around the combined WGS/CO_2 PSA reactor since the specified molar ratio of H_2 to CO of 1.05 in the feed to the first F-T synthesis reactor is already met. Note that the addition of purge gas from the F-T unit to the gasifier increases the H_2/CO ratio in the syngas to above 1.0 which would not be the case with just the bituminous coal feed. The fraction of the syngas shifted is based upon the H_2 demand of the hydrotreating and hydrocracking of the F-T liquids. Syngas leaving the combined WGS/CO_2 PSA reactor is cooled and provided to a PSA unit to provide H_2 required by the F-T liquids processing and the remainder to the F-T synthesis unit.

F-T unit makeup syngas is preheated to 193°C, passed through a bed of ZnO (sandwiching a COS hydrolysis catalyst) to remove the trace amounts of sulfur compounds present, and expanded in a turboexpander from a pressure of 33.6 bar to 23.5 bar as required by the synloop. The turboexpander is connected to the motor assisted synloop recycle compressor. The expanded gas is combined with the synloop recycle gas after the recycle gas is cooled in a series of heat exchangers and treated in an amine wash unit to remove CO_2 to satisfy the required Riblette rato [(FEED H_2 – FEED CO_2)/(FEED CO + FEED CO_2)]of 0.9837 at the reactor inlet. The combined stream is then preheated by a feed/effluent interchanger before being fed to a slurry reactor with Fe based catalyst particles suspending in an inert hydrocarbon liquid (a mineral oil). The mineral oil acts as a temperature moderator and a heat removal medium, transferring the heat of reaction from the catalyst surface via the liquid slurry to boiling water in an internal tubular heat exchanger. IP steam is generated from the heat. The major overall reactions occurring are: $(2n+1)\ H_2 + n\ CO = H\text{-}(CH_2\text{-})_n\text{-}H + n\ H_2O$ and $CO + H_2O = CO_2 + H_2$. The reactor effluent at 253°C is cooled against BFW, in the feed/effluent interchanger and then in a series of heat exchangers to condense out the liquids followed by preheating in a second interchanger before being fed into a second slurry reactor for additional conversion. The effluent from this second rector at 253°C is cooled against BFW, in the feed/effluent interchanger and then in a series of heat exchangers to condense out the liquids. The condensate collected after removing the decanted water is fed to a distillation column operating at 2 bar to remove the light ends, the bottoms from which are then fed to a vacuum column operating at 0.04 bar. The overhead condensate is fed to a hydrotreater to produce the naphtha coproduct while the bottoms are treated in a hydrocracker to produce the diesel coproduct. The overhead vapors from these operations are combined with the PSA tail gas and purge gas and then compressed before being recycled to the gasifier. A fraction of the purge gas is preheated to a temperature of 203ºC and supplied to the gas turbines in the combined cycle unit.

6 Results and Discussion

In this study, performance of the air separation unit, gasifier, AGR as well as 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, vendors be contacted for providing performance and cost data.

6.1 IGCC Cases

Performance summaries for the E-Gas cases are presented in Table 7 and those for the GEP cases are presented in Table 8, while Table 9 and Table 10 summarize the plant cost estimates. The process economics for the two sets of cases are all summarized in Table 11.

In the Cold Gas Cleanup cases, the gas turbine output was shaft limited while inlet air flow limited for the Warm Gas Cleanup cases due to the much higher moisture content of the syngas.

Comparing the two E-Gas cases, the heat rate with the Warm Gas Cleanup employing TDA's combined WGS and CO_2 PSA reactor is 10.3% lower, while at the same time the plant cost on a $/kW is reduced by about 12.7% resulting in a decrease in the COE (with CO_2 TS&M costs included) by about 12.6%. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $26/tonne which is significantly lower than that for the Cold Gas Cleanup case at $43/tonne. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the SCPC (w/o CO_2 capture) for the Warm Gas Cleanup case is $47/tonne, again significantly lower than that for the Cold Gas Cleanup case at $62/tonne. Note that the CH_4 content was allowed to be higher for the warm gas case since percentage carbon capture with TDA's process is higher compared to Selexol™ (gasifier performance for this Warm Gas Cleanup case was estimated by interpolating the performance of the E-Gas gasifier between the two DOE/NETL report cases with and without carbon capture[1]).

Next, comparing the two GEP cases, the heat rate with the Warm Gas Cleanup employing TDA's combined WGS and CO_2 PSA reactor is 8.5% lower, while at the same time the plant cost on a $/kW is reduced by about 6% resulting in a decrease in the COE (with CO_2 TS&M costs included) by about 7.7%. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the corresponding IGCC (w/o CO_2 capture) for the Warm Gas Cleanup case is $28/tonne which is significantly lower than that for the Cold Gas Cleanup case at $38/tonne. The 1st year CO_2 capture cost (without CO_2 TS&M included) compared to the SCPC (w/o CO_2 capture) for the Warm Gas Cleanup case is $54/tonne, again significantly lower than that for the Cold Gas Cleanup case at $61/tonne. Improvement in efficiency over the corresponding Cold Gas Cleanup case is less pronounced when compared to the E-Gas cases because in the Warm Gas Cleanup E-Gas case, the CH_4 content was allowed to be higher.

These 1st year CO_2 capture costs compared to the SCPC without CO_2 capture for the above Warm Gas Cleanup cases are much higher than when compared to the IGCC without CO_2 capture. Note however,

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[1] In the two stage E-Gas™ gasifier, the relative amount of O_2 supplied to each stage may be varied (within limits) to vary the gasifier cold gas efficiency and the syngas composition including its CH_4 content.

that comparison to the SCPC may not be fair since this comparison does not account for the other environmental benefits that the IGCC offers over the SCPC.

6.2 Fischer-Tropsch Cases

Performance summary for the Cold Gas Cleanup and the Warm Gas Cleanup F-T liquids cases are presented in Table 12, while Table 13 summarizes the plant cost for the Cold Gas Cleanup and the Warm Gas Cleanup cases. The process economics for the two cases are summarized in Table 14.

Both the Cold Gas Cleanup and Warm Gas Cleanup cases are designed for the same coal feed rate of 19,053 tonne/D (as received basis) consistent with the reference case summarized in DOE/NETL-2011/1477 which results in the production of 1,475 tonne/D naphtha and 3,632 tonne/D diesel in the Cold Gas Cleanup case, and 1,509 tonne/D naphtha and 3,601 tonne/D diesel in the Warm Gas Cleanup case. With the three GE 6B type gas turbine based combined cycles, the amount of excess power generated is 140 MW in the Cold Gas Cleanup case and as much as 253 MW in the Warm gas Cleanup case due to its higher efficiency. Majority of the power generated in these plants is by the steam turbine. The export power was credited at $59.59/MWh while generating the 1st year required sales price (RSP) for the naphtha and for the diesel using the commercial fuel structure with capital charge factor of 0.218. The total plant cost for the Warm Gas Cleanup case is slightly lower than that of the Cold Gas Cleanup case (by about 1%). However, due to the significantly higher export power of the Warm gas Cleanup case, the RSP of the products is reduced over the Cold Gas Cleanup case. The RSP with CO_2 TS&M included was calculated to be $120/bbl for the naphtha and $172/bbl for the diesel in the case of Cold Gas Cleanup, and $115/bbl for the naphtha and $166/bbl for the diesel in the case of Warm Gas Cleanup, a decrease of more than 3% for each of these coproducts.

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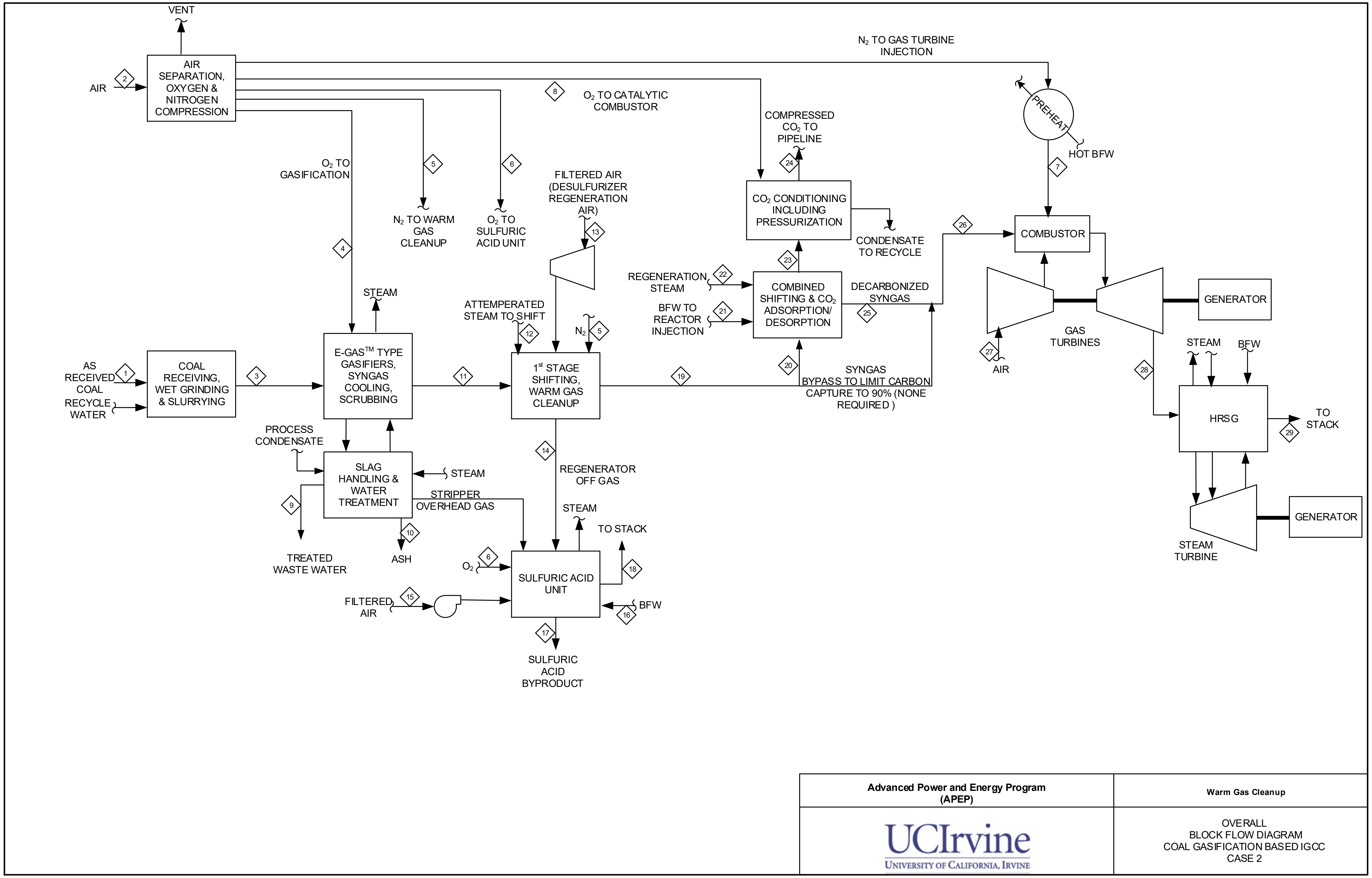


Figure 1. Block Flow Diagram for IGCC System - Case 2 (E-Gas Type Gasifier)

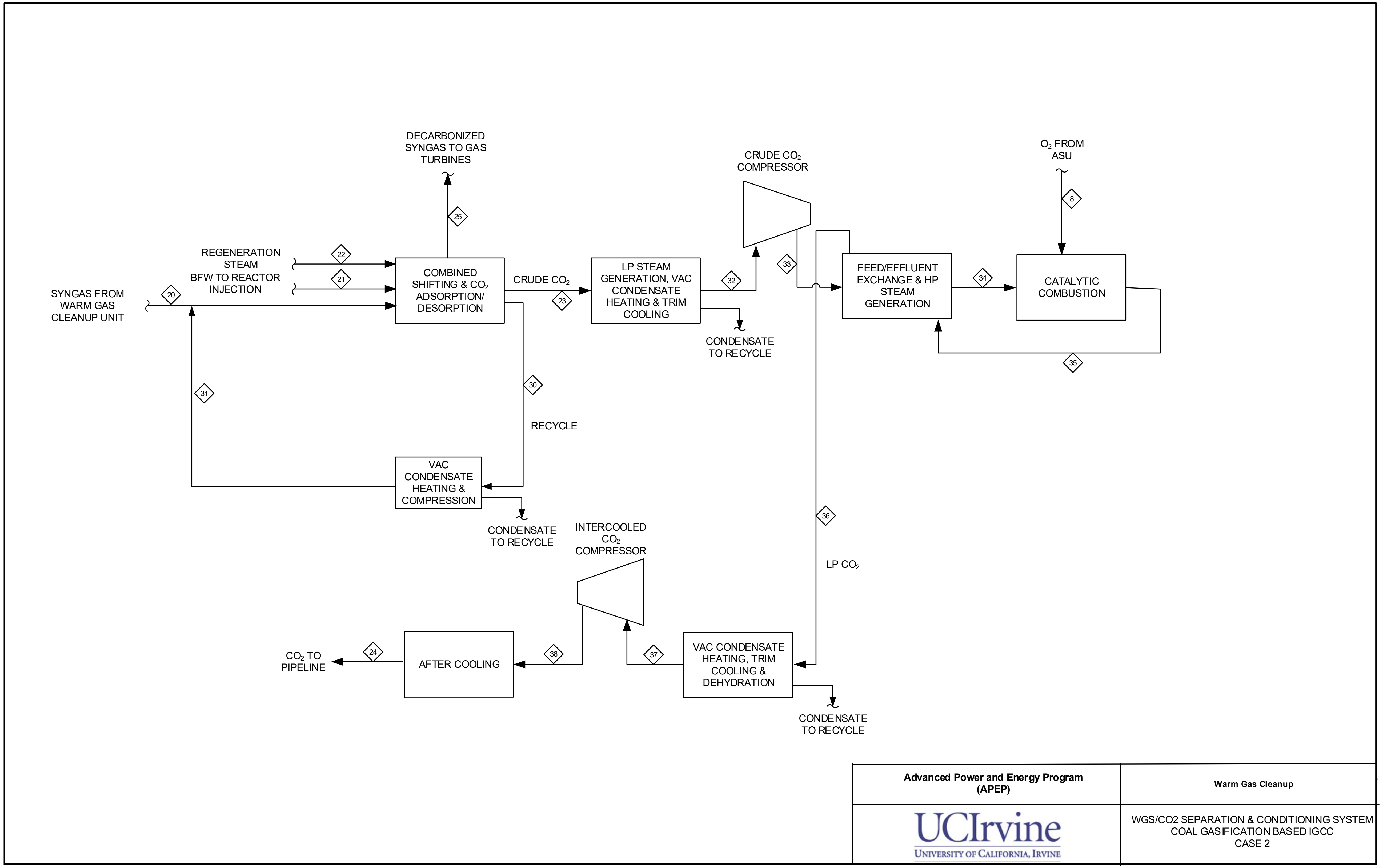


Figure 2. WGS and CO2 PSA System - Case 2 (E-Gas Type Gasifier)

Table 4. Stream Data - Case 2 (E-Gas Type Gasifier)

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Temperature, C	15	15	149	81	60	32	196	145	58	60	185	345	15	760	15	141	20	43	210
Pressure, bar	1.01	1.01	57.92	50.33	41.20	8.62	30.52	20.50	3.10	1.01	38.78	51.02	1.01	34.99	1.01	8.00	1.01	1.01	34.85
Vapor Fraction	-	1.0	-	1.0	1.0	1.0	1.0	1.0	0.0	-	1.0	1.0	1.0	1.0	1.0	-	-	1.0	1.0
Molar Flow, kmol/hr		25,638		5,096	270	100	11,110	163	With Solids	Dry Basis	28,727	0	1,265	1,441	505	162	169	1,796	26,943
Mass Flow, kg/hr	212,637	739,707	299,986	164,023	7,569	3,228	311,793	5,240	26,830	21,703	584,439	0	36,506	46,538	14,570	2,917	16,301	51,047	545,499
Fluid Avg Mol Wt		28.9	18.0	32.2	28.1	32.2	28.1	32.2	18.0	-	20.3	18.0	28.8	32.3	28.9	18.0	96.5	28.4	20.2
Fluid Mole Fractions																			
O2		0.21		0.95	0.01	0.95	0.01	0.95			0.00	-	0.21	0.01	0.21	-	-	0.07	0.00
N2		0.77		0.02	0.99	0.02	0.99	0.02			0.01	-	0.77	0.86	0.77	-	-	0.91	0.01
AR		0.01		0.03	0.00	0.03	0.00	0.03			0.01	-	0.01	0.01	0.01	-	-	0.01	0.01
H2		-		-	-	-	-	-			0.25	-	-	-	-	-	-	-	0.42
CO		-		-	-	-	-	-			0.26	-	-	-	-	-	-	-	0.08
CO2		0.00		-	-	-	-	-			0.13	-	0.00	0.00	0.00	-	-	0.00	0.31
H2O		0.01		-	0.00	-	0.00	-	1.00		0.32	1.00	0.01	0.00	0.01	1.00	0.02	0.00	0.15
CH4		-		-	-	-	-	-			0.03	-	-	-	-	-	-	-	0.03
H2S		-		-	-	-	-	-			0.01	-	-	-	-	-	-	-	0.00
NH3		-		-	-	-	-	-			0.00	-	-	-	-	-	-	-	0.00
CL2		-		-	-	-	-	-			0.00	-	-	-	-	-	-	-	0.00
HCN		-		-	-	-	-	-			-	-	-	-	-	-	-	-	-
SO2		-		-	-	-	-	-			-	-	-	-	-	-	-	-	-
H2SO4		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.98	-	-
Total		1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00	0.89	1.00	1.00	1.00	1.00	1.00

Table 4. Stream Data (Cont'd) - Case 2 (E-Gas Type Gasifier)

Stream No.	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38
Temperature, C	210	141	205	186	27	203	203	15	567	300	228	178	27	90	288	435	135	27	27
Pressure, bar	34.85	144.79	10.34	10.34	152.70	32.89	32.89	1.01	1.05	0.99	9.89	34.65	9.58	20.00	19.79	19.10	18.55	17.79	152.70
Vapor Fraction	1.0	-	1.0	1.0	-	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-
Molar Flow, kmol/hr	26,927	1,818	9,755	17,921	10,091	20,334	20,350	109,670	134,485	134,485	2,991	2,745	10,310	10,310	10,324	10,358	10,358	10,085	10,085
Mass Flow, kg/hr	545,165	32,759	175,743	580,419	443,972	168,823	169,157	3,163,970	3,644,920	3,644,920	82,146	77,721	443,336	443,336	443,549	448,789	448,789	443,794	443,794
Fluid Avg Mol Wt	20.2	18.0	18.0	32.4	44.0	8.3	8.3	28.8	27.1	27.1	27.5	28.3	43.0	43.0	43.0	43.3	43.3	44.0	44.0
Fluid Mole Fractions																			
O2	0.00	-	-	0.00	0.00	0.00	0.00	0.21	0.11	0.11	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N2	0.01	-	-	0.00	0.00	0.01	0.01	0.77	0.71	0.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-
AR	0.01	-	-	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.42	-	-	0.01	0.00	0.64	0.64	-	-	-	0.32	0.35	0.02	0.02	0.02	-	-	0.00	0.00
CO	0.08	-	-	0.00	0.00	0.01	0.01	-	-	-	0.01	0.01	0.00	0.00	0.00	-	-	0.00	0.00
CO2	0.31	-	-	0.56	1.00	0.01	0.01	0.00	0.01	0.01	0.56	0.61	0.97	0.97	0.97	0.97	0.97	1.00	1.00
H2O	0.15	1.00	1.00	0.42	-	0.29	0.29	0.01	0.16	0.16	0.09	0.01	0.00	0.00	0.00	0.03	0.03	-	-
CH4	0.03	-	-	0.00	-	0.03	0.03	-	-	-	0.02	0.02	-	-	0.00	-	-	-	-
H2S	0.00	-	-	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00	0.00	-	-	0.00	0.00
NH3	0.00	-	-	0.00	-	-	0.00	-	0.00	0.00	-	-	-	-	-	-	-	-	-
CL2	0.00	-	-	0.00	0.00	0.00	0.00	-	-	-	-	-	0.00	0.00	0.00	-	-	0.00	0.00
HCN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
SO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2SO4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

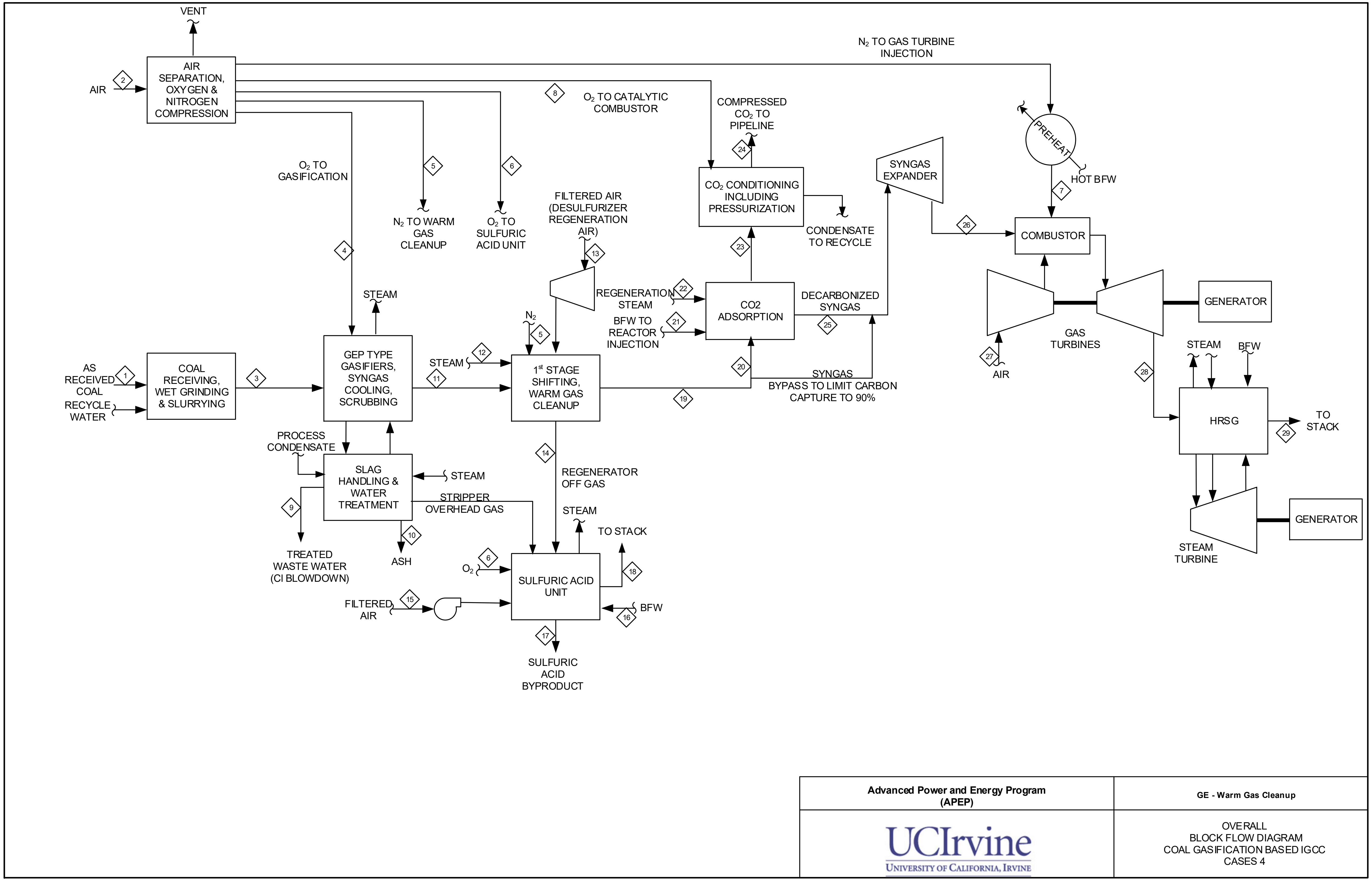

VENT
AIR
2
AIR SEPARATION, OXYGEN & NITROGEN COMPRESSION
N₂ TO GAS TURBINE INJECTION
8
O₂ TO CATALYTIC COMBUSTOR
COMPRESSED CO₂ TO PIPELINE
24
O₂ TO GASIFICATION
5
6
N₂ TO WARM GAS CLEANUP
O₂ TO SULFURIC ACID UNIT
4
FILTERED AIR (DESULFURIZER REGENERATION AIR)
13
CO₂ CONDITIONING INCLUDING PRESSURIZATION
CONDENSATE TO RECYCLE
23
SYNGAS EXPANDER
PREHEAT
HOT BFW
7
26
COMBUSTOR
STEAM
N₂
5
REGENERATION STEAM
22
BFW TO REACTOR INJECTION
21
CO2 ADSORPTION
DECARBONIZED SYNGAS
25
GAS TURBINES
GENERATOR
27
AIR
AS RECEIVED COAL
1
RECYCLE WATER
COAL RECEIVING, WET GRINDING & SLURRYING
3
GEP TYPE GASIFIERS, SYNGAS COOLING, SCRUBBING
STEAM
12
11
1st STAGE SHIFTING, WARM GAS CLEANUP
20
19
SYNGAS BYPASS TO LIMIT CARBON CAPTURE TO 90%
STEAM
BFW
28
HRSG
TO STACK
29
PROCESS CONDENSATE
SLAG HANDLING & WATER TREATMENT
STEAM
STRIPPER OVERHEAD GAS
9
10
ASH
TREATED WASTE WATER (CI BLOWDOWN)
14
REGENERATOR OFF GAS
STEAM
TO STACK
18
O₂
6
SULFURIC ACID UNIT
FILTERED AIR
15
BFW
16
17
SULFURIC ACID BYPRODUCT
STEAM TURBINE
GENERATOR
Advanced Power and Energy Program (APEP)
GE - Warm Gas Cleanup
UCIrvine
UNIVERSITY OF CALIFORNIA, IRVINE
OVERALL BLOCK FLOW DIAGRAM COAL GASIFICATION BASED IGCC CASES 4

Figure 3. Case 4 (GEP Type Gasifier) - Block Flow Diagram for IGCC System

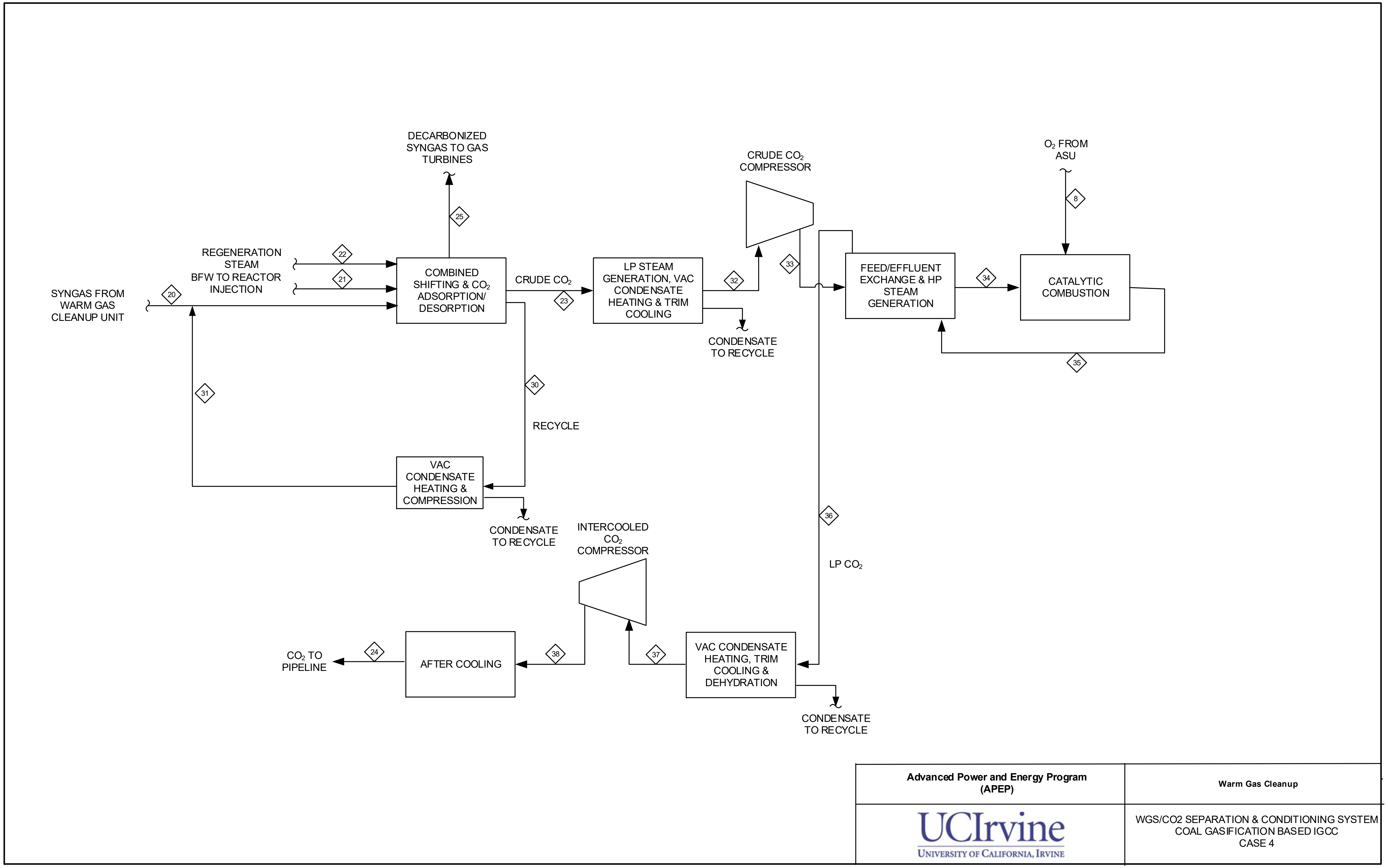


Figure 4. Case 4 (GEP Type Gasifier) – WGS and CO2 PSA System

Table 5. Case 4 (GEP Type Gasifier) – Stream Data

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Temperature, C	15	15	77	93	60	32	196	145	57	60	206	404	15	760	15	141	20	43	198
Pressure, bar	1.01	1.01	72.39	64.81	41.20	8.62	30.52	20.50	3.10	1.01	53.61	56.19	1.01	39.82	1.01	8.00	1.01	1.01	50.16
Vapor Fraction	-	1.0	-	1.0	1.0	1.0	1.0	1.0	0.0	-	1.0	1.0	1.0	1.0	1.0	-	-	1.0	1.0
Molar Flow, kmol/hr		26,396		5,330	270	101	7,903	129	With Solids	Dry Basis	30,522	0	1,267	1,443	506	131	169	1,794	30,514
Mass Flow, kg/hr	213,013	761,587	300,518	171,542	7,577	3,238	221,780	4,152	27,232	23,371	596,654	2	36,548	46,592	14,608	2,356	16,329	50,929	593,844
Fluid Avg Mol Wt		28.9	18.0	32.2	28.1	32.2	28.1	32.2	18.0	-	19.5	18.0	28.8	32.3	28.9	18.0	96.5	28.4	19.5
Fluid Mole Fractions																			
O2		0.21		0.95	0.01	0.95	0.01	0.95			7.23E-14	-	0.21	0.01	0.21	-	-	0.06	7.23E-14
N2		0.77		0.02	0.99	0.02	0.99	0.02			0.01	-	0.77	0.86	0.77	-	-	0.92	0.01
AR		0.01		0.03	0.00	0.03	0.00	0.03			0.01	-	0.01	0.01	0.01	-	-	0.01	0.01
H2		-		-	-	-	-	-			0.25	-	-	-	-	-	-	-	0.44
CO		-		-	-	-	-	-			0.26	-	-	-	-	-	-	-	0.07
CO2		0.00		-	-	-	-	-			1.01E-01	0.00E+00	3.00E-04	2.63E-04	3.00E-04	0.00E+00	0.00E+00	0.00	0.29
H2O		0.01		-	1.84E-13	-	1.88E-13	-	1.00		3.71E-01	1.00E+00	1.08E-02	1.79E-03	1.04E-02	1.00E+00	2.01E-02	0.00	0.19
CH4		-		-	-	-	-	-			8.33E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-	0.00
H2S		-		-	-	-	-	-			0.01	-	-	-	-	-	-	-	1.08E-05
NH3		-		-	-	-	-	-			0.00	-	-	-	-	-	-	-	0.00
CL2		-		-	-	-	-	-			0.00	-	-	-	-	-	-	-	1.08E-07
HCN		-		-	0.00E+00	-	0.00E+00	-			-	-	-	-	-	-	-	-	-
SO2		-		-	0.00E+00	-	0.00E+00	-			-	-	-	-	-	-	-	-	-
H2SO4		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.98	-	-
Total		1.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00	0.88	1.00	1.00	1.00	1.00	1.00

Table 5. Case 4 (GEP Type Gasifier) – Stream Data (Cont'd)

Stream No.	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38
Temperature, C	198	141	220	186	27	203	195	15	569	153	235	218	27	90	288	410	135	27	27
Pressure, bar	50.16	144.79	10.34	10.34	152.70	47.90	31.72	1.01	1.05	0.99	10.11	49.47	9.58	20.00	19.79	19.10	18.55	17.79	152.70
Vapor Fraction	1.0	-	1.0	1.0	-	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	-
Molar Flow, kmol/hr	28,622	1,793	7,381	16,001	9,983	21,407	23,300	109,472	133,024	133,024	3,924	3,537	10,222	10,222	10,222	10,230	10,230	9,983	9,983
Mass Flow, kg/hr	557,013	32,307	132,970	543,625	439,236	171,691	208,521	3,158,246	3,588,548	3,588,548	110,187	103,213	439,526	439,526	439,532	443,684	443,684	439,236	439,236
Fluid Avg Mol Wt	19.5	18.0	18.0	34.0	44.0	8.0	8.9	28.8	27.0	27.0	28.1	29.2	43.0	43.0	43.0	43.4	43.4	44.0	44.0
Fluid Mole Fractions																			
O2	7.23E-14	-	-	1.99E-15	8.55E-06	9.52E-14	9.34E-14	0.21	0.11	0.11	-	-	-	-	3.11E-15	8.34E-06	8.34E-06	8.55E-06	8.55E-06
N2	0.01	-	-	0.00	0.00	0.01	0.01	0.77	0.70	0.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AR	0.01	-	-	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.44	-	-	0.01	2.11E-08	0.66	0.64	-	-	-	0.31	0.34	0.02	0.02	0.02	-	-	2.11E-08	2.11E-08
CO	0.07	-	-	0.00	3.25E-09	0.01	0.01	-	-	-	0.00	0.00	0.00	0.00	0.00	-	-	3.25E-09	3.25E-09
CO2	0.29	-	-	0.62	9.99E-01	9.22E-03	0.03	0.00	0.01	0.01	5.72E-01	0.63	0.97	9.72E-01	9.72E-01	9.75E-01	9.75E-01	9.99E-01	9.99E-01
H2O	0.19	1.00	1.00	0.36	0.00E+00	3.05E-01	0.30	0.01	0.17	0.17	1.06E-01	0.01	0.00	3.45E-03	3.45E-03	2.41E-02	2.41E-02	0.00E+00	0.00E+00
CH4	0.00	-	-	2.49E-05	0.00E+00	1.10E-03	0.00	-	-	-	5.14E-04	0.00	-	0.00E+00	3.89E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
H2S	1.08E-05	-	-	3.22E-07	5.16E-13	1.43E-05	1.40E-05	-	-	-	6.71E-06	7.45E-06	5.04E-07	5.04E-07	5.04E-07	-	0.00E+00	5.16E-13	5.16E-13
NH3	0.00	-	-	0.00	-	-	6.80E-05	-	1.19E-05	1.19E-05	-	-	-	-	-	-	0.00E+00	0.00E+00	-
CL2	1.08E-07	-	-	2.96E-09	4.75E-15	2.12E-08	2.82E-08	-	-	-	-	-	4.63E-09	4.63E-09	4.63E-09	-	0.00E+00	4.75E-15	4.75E-15
HCN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.00E+00	0.00E+00	-
SO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.00E+00	0.00E+00	-
H2SO4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

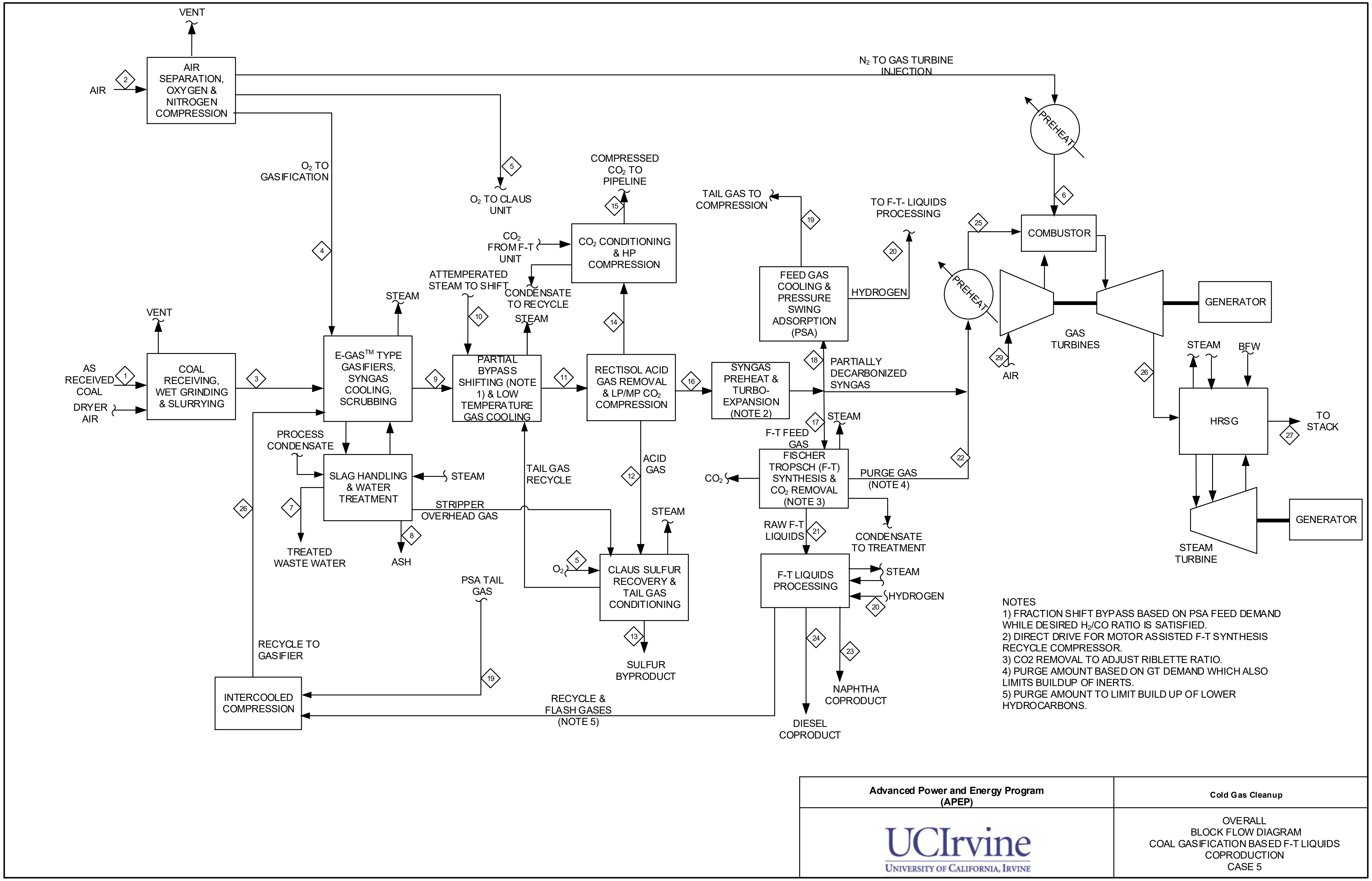
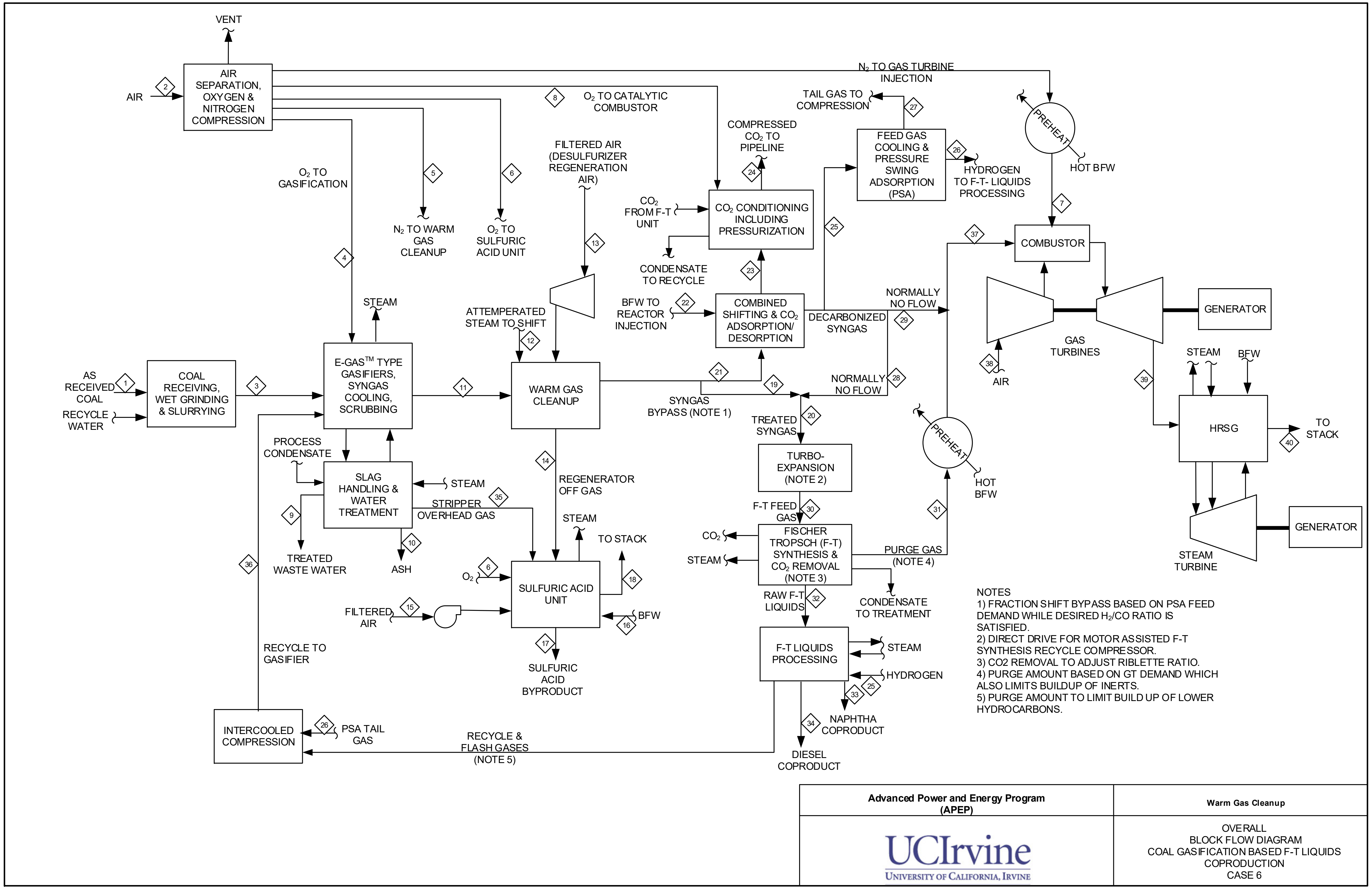


Figure 5. Case 5 (E-Gas Type Gasifier) - Block flow diagram with Cold Gas Cleanup for F-T Liquids



NOTES
1) FRACTION SHIFT BYPASS BASED ON PSA FEED DEMAND WHILE DESIRED H_2/CO RATIO IS SATISFIED.
2) DIRECT DRIVE FOR MOTOR ASSISTED F-T SYNTHESIS RECYCLE COMPRESSOR.
3) CO2 REMOVAL TO ADJUST RIBLETTE RATIO.
4) PURGE AMOUNT BASED ON GT DEMAND WHICH ALSO LIMITS BUILDUP OF INERTS.
5) PURGE AMOUNT TO LIMIT BUILD UP OF LOWER HYDROCARBONS.

Figure 6. Case 6 (E-Gas Type Gasifier) - Block flow diagram with Warm Gas Cleanup for F-T Liquids

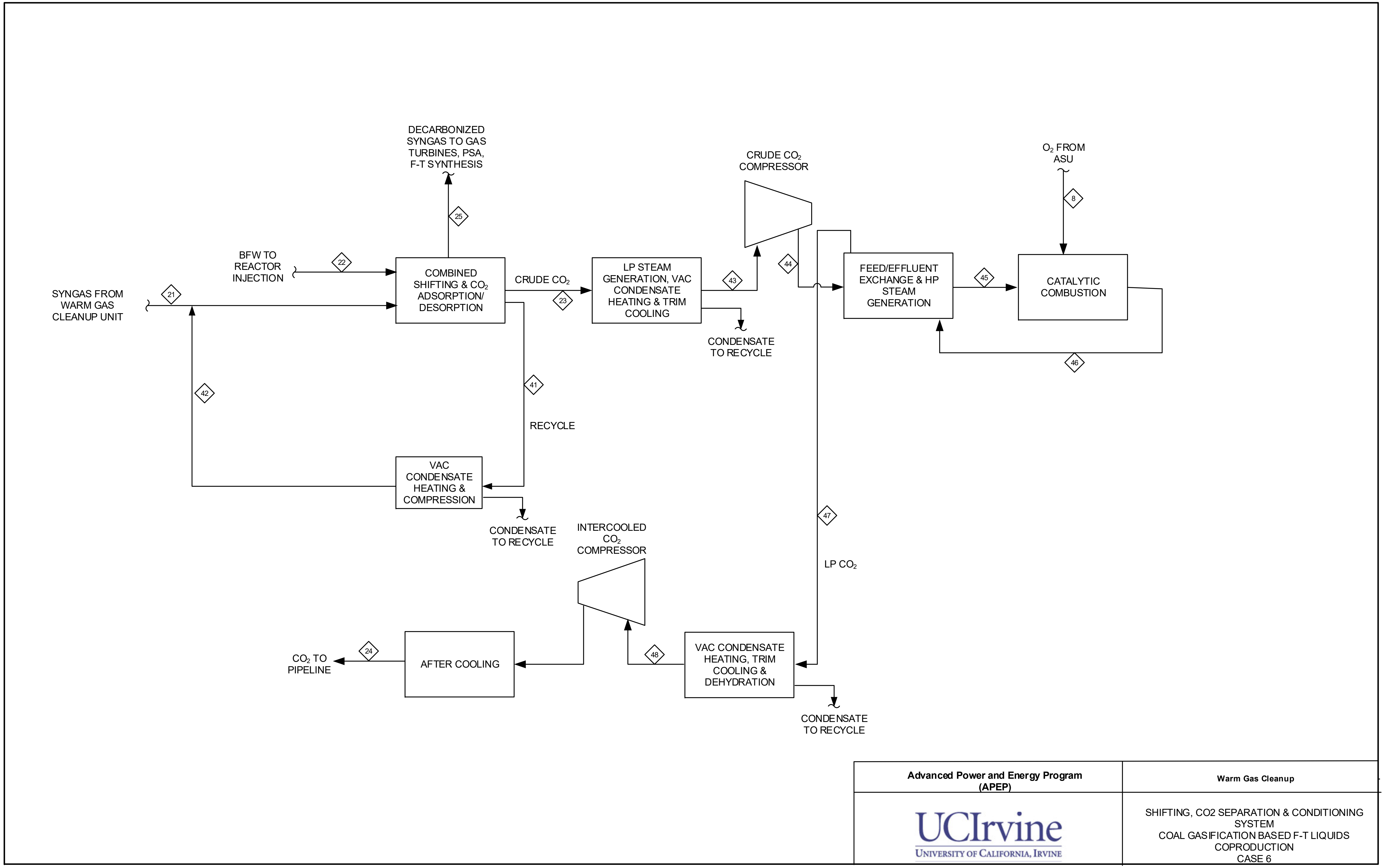


Figure 7. Case 6 (E-Gas Type Gasifier) – WGS and CO2 PSA System

Table 6. Case 6 (E-Gas Type Gasifier) – Stream Data

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
Temperature, C	15	-	149	88	60	19	196	145	54	-	184	392	15	760	15	141	20	43	202	201	202	141	186	27
Pressure, bar	1.01	-	57.92	50.33	41.20	8.58	30.52	20.50	3.10	1.01	38.78	51.02	1.01	35.68	1.01	8.00	1.01	1.01	36.37	32.89	36.37	144.79	10.34	152.70
Vapor Fraction	-	-	-	1.0	1.0	1.0	1.0	1.0	0.0	-	1.0	1.0	1.0	1.0	1.0	-	-	1.0	1.0	1.0	1.0	-	1.0	-
Fluid Molar Flow, kmol/hr		0		19,306	519	374	3,575	51	With Solids	Dry Basis	128,668	0	5,222	5,386	1,886	601	798	6,949	117,274	117,277	3,273	781	2,139	23,200
Mass Flow, kg/hr	793,864	0	1,119,978	621,381	14,564	12,050	100,334	1,638	100,849	81,028	2,579,302	2	150,667	174,350	54,411	10,823	63,862	193,869	2,341,653	2,341,683	65,361	14,064	69,449	1,021,011
Fluid Avg Mol Wt		-	18.0	32.2	28.1	32.2	28.1	32.2	18.0	-	20.0													
Fluid Mole Fractions																								
O2		0.00		0.95	0.01	0.95	0.01	0.95			0.00	0.00	0.21	0.03	0.21	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00
N2		0.00		0.02	0.99	0.02	0.99	0.02			0.01	0.00	0.77	0.84	0.77	0.00	0.00	0.89	0.01	0.01	0.01	0.00	0.00	0.00
AR		0.00		0.03	0.00	0.03	0.00	0.03			0.02	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.02	0.02	0.02	0.00	0.00	0.00
H2		0.00		0.00	0.00	0.00	0.00	0.00			0.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.26	0.26	0.00	0.01	0.00
CO		0.00		0.00	0.00	0.00	0.00	0.00			0.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.26	0.26	0.00	0.00	0.00
CO2		0.00		0.00	0.00	0.00	0.00	0.00			0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.12	0.12	0.00	0.56	1.00
H2O		0.00		0.00	0.00	0.00	0.00	0.00	1.00		0.31	1.00	0.01	0.00	0.01	1.00	0.22	0.05	0.32	0.32	0.32	1.00	0.43	0.00
CH4		0.00		0.00	0.00	0.00	0.00	0.00			0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.00	0.00	0.00
H2S		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NH3		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
HCN		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3H8		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4H10		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5H12		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9H20		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9H18		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C15H32		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C15H30		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C20H40		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C21H44		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C30H60		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CH3OH		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00		0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total		0.00		1.00	1.00	1.00	1.00	1.00	1.00		1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 6. Case 6 (E-Gas Type Gasifier) – Stream Data (Cont'd)

Stream No.	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
Temperature, C	203	38	33	203	203	172	55	55	28	37	27	170	109	15	553	174	228	179	29	97	288	307	140	27
Pressure, bar	32.89	32.55	1.36	32.89	32.89	23.50	23.50	3.00	1.72	1.72	2.07	50.00	23.50	1.01	1.05	0.99	9.89	34.65	9.24	20.00	19.79	19.10	18.55	17.79
Vapor Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.1	-	-	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Fluid Molar Flow, kmol/hr	3,005	1,443	385	3	3	116,860	5,117	1,227	397	713	332	11,883	8,695	40,383	48,083	48,083	402	337	23,329	23,329	23,330	23,357	23,357	23,200
Mass Flow, kg/hr	29,652	4,287	4,171	30	30	2,334,548	112,540	237,717	62,887	150,061	5,906	252,290	212,904	1,165,040	1,377,944	1,377,944	10,584	9,411	1,022,231	1,022,230	1,022,241	1,023,879	1,023,879	1,021,011
Fluid Avg Mol Wt																								
Fluid Mole Fractions																								
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.21	0.11	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N2	0.01	0.00	0.09	0.01	0.01	0.01	0.08			0.00	0.00	0.08	0.46	0.77	0.73	0.73	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
AR	0.02	0.02	0.04	0.02	0.02	0.02	0.11			0.00	0.00	0.10	0.07	0.01	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.55	0.97	0.64	0.55	0.55	0.26	0.39			0.00	0.00	0.42	0.23	0.00	0.00	0.00	0.31	0.36	0.00	0.00	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.04	0.00	0.00	0.26	0.04			0.00	0.00	0.04	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.01	0.00	0.05	0.01	0.01	0.12	0.24			0.00	0.01	0.22	0.14	0.00	0.05	0.05	0.50	0.59	0.99	0.99	0.99	0.99	0.99	1.00
H2O	0.39	0.00	0.01	0.39	0.39	0.32	0.00			0.00	0.00	0.00	0.00	0.01	0.08	0.08	0.17	0.01	0.00	0.00	0.00	0.01	0.01	0.00
CH4	0.02	0.00	0.13	0.02	0.02	0.02	0.12			0.00	0.00	0.12	0.07	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
H2S	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NH3	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCN	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3H8	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4H10	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5H12	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9H20	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9H18	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C15H32	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C15H30	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C20H40	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C21H44	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C30H60	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CH3OH	0.00	0.00	0.00	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 7. Performance Summary – E-Gas Type Gasifier based IGCC Cases

CASE	**1**
GASIFIER TYPE	**E-Gas**
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	464,000
STEAM TURBINE POWER	244,875
SYNGAS EXPAMDER	
TOTAL POWER, kW	708,875
AUXILIARY LOAD SUMMARY, kW	
COAL HANDLING	448
COAL GRINDING	2,269
COAL SLURRY PUMPS	629
SLAG/ASH HANDLING & DEWATERING	1,118
AIR SEPARATION UNIT AUXILIARIES	1,071
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	65,689
OXYGEN COMPRESSOR	9,125
NITROGEN COMPRESSOR	34,536
SYNGAS RECYCLE COMPRESSOR	1,275
TAIL GAS RECYCLE COMPRESSOR	5,396
CO2 COMPRESSOR	31,543
BOILER FEEDWATER & DEMIN PUMPS	5,431
VACUUM CONDENSATE PUMP	368
PROCESS CONDENSATE & SWS SYSTEMS	51
HUMIDIFIER & BFW CIRCULATING PUMPS	44
COOLING WATER CIRCULATING PUMPS	4,956
COOLING TOWER FANS	2,502
AIR COOLED CONDENSER FANS	
SCRUBBER PUMPS	396
SELEXOL UNIT	20,999
GAS TURBINE AUXILIARIES	1,000
STEAM TURBINE AUXILIARIES	107
CLAUS & TAIL GAS TREATING AUXILIARIES	204
MISCELLANEOUS BALANCE OF PLANT	3,053
TRANSFORMER LOSSES	2,626
TOTAL AUXIIARIES, kW	194,835
NET POWER, kW	514,040
NET PLANT EFFICIENCY, % HHV	30.91
NET HEAT RATE	
kJ/kWh	11,648
BTU/kWh	11,040
CONDENSER COOLING DUTY	
10^6 kJ/h	1,332.39
10^6 BTU/h	1,262.86
CONSUMABLES	
AS-RECEIVED COAL FEED	
kg/h	220,518
lb/h	486,242
THERMAL INPUT, KWT HHV	
RAW WATER USAGE	
M^3/MIN	21.41
GPM	5,657.13
CARBON CAPTURED	
%	90.24
tonne CO2/tonne dry coal	2.353

CASE	**2**
GASIFIER TYPE	**E-Gas**
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	428,558
STEAM TURBINE POWER	264,784
SYNGAS EXPANDER POWER	
TOTAL POWER, KWE	693,342
AUXILIARY LOAD SUMMARY, kW	
COAL HANDLING	432
COAL GRINDING	2,188
COAL SLURRY PUMPS	632
SLAG HANDLING & DEWATERING	1,086
AIR SEPARATION UNIT AUXILIARIES	1,033
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	52,410
OXYGEN COMPRESSOR	13,549
NITROGEN COMPRESSOR	21,682
SYNGAS RECYCLE COMPRESSOR	1,194
CO2 PURIFICATION & COMPRESSION	25,617
BOILER FEEDWATER & DEMIN PUMPS	5,299
VACUUM CONDENSATE PUMP	361
PROCESS CONDENSATE & SWS SYSTEMS	82
BFW CIRCULATING PUMPS	3
COOLING WATER CIRCULATING PUMPS	4,731
COOLING TOWER FANS	2,389
AIR COOLED CONDENSER FANS	
SCRUBBER PUMPS	381
DESULFURIZER UNIT	4,795
GAS TURBINE AUXILIARIES	924
STEAM TURBINE AUXILIARIES	115
H2SO4 UNIT	(3,601)
MISCELLANEOUS BALANCE OF PLANT	2,944
TRANSFORMER LOSSES	2,568
TOTAL AUXIIARIES, kW	140,812
NET POWER, kW	552,529
NET PLANT EFFICIENCY, % HHV	34.45
NET HEAT RATE	
kJ/kWh	10,449
BTU/kWh	9,904
CONDENSER COOLING DUTY	
10^6 kJ/h	1,476
10^6 BTU/h	1,399
CONSUMABLES	
AS-RECEIVED COAL FEED	
kg/h	212,637
lb/h	468,864
THERMAL INPUT, KWT HHV	1,603,713
RAW WATER USAGE	
M^3/MIN	21.52
GPM	5,685
CARBON CAPTURED	
%	90.00
tonne CO2/tonne dry coal	2.346

Table 8. Performance Summary – GEP Type Gasifier based IGCC Cases

CASE	**3**
GASIFIER TYPE	**GEP**
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	464,000
STEAM TURBINE POWER	259,517
SYNGAS EXPAMDER	6,189
TOTAL POWER, kW	729,705
AUXILIARY LOAD SUMMARY, kW	
COAL HANDLING	452
COAL GRINDING	2,292
COAL SLURRY PUMPS	797
SLAG/ASH HANDLING & DEWATERING	1,137
AIR SEPARATION UNIT AUXILIARIES	1,100
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	68,069
OXYGEN COMPRESSOR	10,763
NITROGEN COMPRESSOR	36,046
SYNGAS RECYCLE COMPRESSOR	-
TAIL GAS RECYCLE COMPRESSOR	1,694
CO2 COMPRESSOR	31,418
BOILER FEEDWATER & DEMIN PUMPS	4,739
VACUUM CONDENSATE PUMP	336
PROCESS CONDENSATE & SWS SYSTEMS	231
HUMIDIFIER & BFW CIRCULATING PUMPS	25
COOLING WATER CIRCULATING PUMPS	5,520
COOLING TOWER FANS	2,787
SCRUBBER PUMPS	72
SELEXOL UNIT	19,251
GAS TURBINE AUXILIARIES	1,000
STEAM TURBINE AUXILIARIES	113
CLAUS & TAIL GAS TREATING AUXILIARIES	206
MISCELLANEOUS BALANCE OF PLANT	3,084
TRANSFORMER LOSSES	2,703
TOTAL AUXIIARIES, kW	193,833
NET POWER, kW	535,872
NET PLANT EFFICIENCY, % HHV	31.90
NET HEAT RATE,	
kJ/kWh	11,285
BTU/kWh	10,696
CONDENSER COOLING DUTY	
10^6 kJ/h	1,554
10^6 BTU/h	1,473
CONSUMABLES	
AS-RECEIVED COAL FEED	
KG/h	222,733
lb/h	491,126
THERMAL INPUT, KWT HHV	1,679,861
RAW WATER USAGE	
M^3/MIN	22.38
GPM	5,913
CARBON CAPTURED	
%	90.31
tonne CO2/tonne dry coal	2.326

CASE	**4**
GASIFIER TYPE	**GEP**
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	418,408
STEAM TURBINE POWER	267,865
SYNGAS EXPANDER POWER	8,822
TOTAL POWER, KWE	695,094
AUXILIARY LOAD SUMMARY, KWE	
COAL HANDLING	432
COAL MILLING	2,192
COAL SLURRY PUMPS	722
SLAG HANDLING & DEWATERING	1,088
AIR SEPARATION UNIT AUXILIARIES	440
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	48,426
OXYGEN COMPRESSOR	17,757
NITROGEN COMPRESSOR	15,593
SYNGAS RECYCLE COMPRESSOR	-
CO2 PURIFICATION & COMPRESSION	28,079
BOILER FEEDWATER & DEMIN PUMPS	4,485
VACUUM CONDENSATE PUMP	308
PROCESS CONDENSATE & SWS SYSTEMS	504
BFW CIRCULATING PUMPS	6
COOLING WATER CIRCULATING PUMPS	4,937
COOLING TOWER FANS	2,492
AIR COOLED CONDENSER FANS	
SCRUBBER PUMPS	69
DESULFURIZER UNIT	4,800
GAS TURBINE AUXILIARIES	902
STEAM TURBINE AUXILIARIES	117
H2SO4 UNIT	(3,771)
MISCELLANEOUS BALANCE OF PLANT	2,949
TRANSFORMER LOSSES	2,575
TOTAL AUXIIARIES, KWE	135,100
NET POWER, KWE	559,994
NET PLANT EFFICIENCY, % HHV	34.86
NET HEAT RATE	
KJ/KWH	10,328
BTU/KWH	9,789
CONDENSER COOLING DUTY	
10^6 KJ/H	1,501
10^6 BTU/H	1,422
CONSUMABLES	
AS-RECEIVED COAL FEED	
KG/H	213,013
LB/H	469,694
THERMAL INPUT, KWT HHV	1,606,553
RAW WATER USAGE	
M^3/MIN	21.54
GPM	5,691
CARBON CAPTURED	
%	89.99
tonne CO2/tonne dry coal	2.318

Table 9. Plant Cost Summary – E-Gas Type Gasifier based IGCC Cases

CASE	**1**
ASU	273,006
Fuel receiving, preparation & feeding	112,045
Gasifier, syngas cooler & auxiliaries	311,129
Gasification foundations	21,404
Ash handling systems	45,150
Flare stack system	3,707
Shift reactors	15,875
LTGC & Syngas Humidification	51,143
Blowback gas systems	1,638
Fuel gas piping	1,930
Gas cleanup foundations	1,942
Hg Removal	3,689
Selexol	243,545
Claus & TG Recycle	40,533
CO2 compression & dehydration	67,009
Gas turbine , generator & auxiliaries	159,009
HRSG, ducting & stack	54,095
Steam turbine, generator & auxiliaries	81,508
Steam Condenser	5,604
Feedwater system	20,082
Water makeup + pretreating	2,336
Other feedwater subsystems	4,112
Service water systems	7,113
Other boiler plant systems	8,300
Fuel oil system & nat gas	2,297
Waste water treatment	2,705
Misc. power plant equipment	3,050
Cooling water system	39,997
Accessory electric plant	106,463
Instrumentationo & controls	32,460
Improvement to site	23,158
Buildings & structures	21,692
Total	1,767,721
Specific plant cost, $/kW	**3,439**

CASE	**2**
ASU	263,327
Fuel receiving, preparation & feeding	109,386
Gasifier, syngas cooler & auxiliaries	302,531
Gasification foundations	21,018
Ash handling systems	44,255
Flare stack system	3,640
Warm gas desulfurization	33,528
H2SO4 unit	73,878
Shift reactor & heat exchange	6,211
Blowback gas systems	1,620
Fuel gas piping	2,262
Gas cleanup foundations	1,524
Trace contaminant removal	4,206
WGS/CO2 PSA	129,110
CO2 purification & heat recovery	28,917
CO2 compression & drying	59,380
Gas turbine, generator & auxiliaries	159,009
HRSG, ducting & stack	53,128
Steam turbin, generator & auxiliaries	86,091
Steam condenser	6,027
Feedwater system	17,503
Water makeup & pretreating	2,345
Other feedwater subsystems	4,347
Service water systems	6,931
Other boiler plant systems	8,787
Fuel oil system & nat gas	2,254
Waste water treatment	2,636
Misc. power plant equipment	3,034
Cooling water system	38,680
Accessory electric plant	105,407
Instrumentationo & controls	32,307
Improvement to site	23,090
Buildings & structures	21,613
Total	1,657,979
Specific plant cost, $/kW	**3,001**

Table 10. Plant Cost Summary – GEP Type Gasifier based IGCC Cases

CASE	**3**
ASU	284,065
Fuel receiving, preparation & feeding	115,143
Gasifier, syngas cooler & auxiliaries	310,284
Gasification foundations	19,084
Ash handling	55,505
Soot Recovery + SARU	7,056
Shift reactors	22,137
Syngas scrubber + LTGC	26,440
Fuel gas piping	1,752
Gas cleanup foundations	1,821
Hg Removal	4,161
Selexol	257,485
Claus & TG Recycle	40,805
CO2 compression, dehydration & pumping	66,885
Syngas Expander	9,236
Gas turbine, generator & auxiliaries	159,299
HRSG, ducting & stack	54,241
Steam turbine, generator & auxiliaries	84,133
Surface condenser	6,136
Feedwater system	19,332
Water makeup & pretreating	2,400
Other feedwater subsystems	4,009
Service water systems	7,221
Other boiler plant systems	8,180
Fuel oil system & nat gas	2,315
Waste water treatment	2,745
Misc. power plant equipment	3,118
Cooling water system	43,036
Accessory electric plant	106,607
Instrumentationo & controls	33,222
Improvement to site	23,634
Buildings & structures	22,356
Total	1,803,840
Specific plant cost, $/kW	**3,366**

CASE	**4**
ASU	285,214
Fuel receiving, preparation & feeding	111,801
Gasifier, syngas cooler & auxiliaries	299,804
Gasification foundations	18,662
Ash handling systems	54,160
Soot Recovery & SARU	6,900
Warm gas desulfurization	33,575
H2SO4 unit	73,966
Shift reactor & heat exchange	9,210
Syngas scrubber	11,076
Fuel gas piping	2,161
Gas cleanup foundations	1,518
Trace contaminant removal	4,247
WGS/CO2 PSA	153,182
CO2 purification & heat recovery	48,373
CO2 compression & drying	63,162
Syngas Expander	11,838
Gas turbine, generator & auxiliaries	159,299
HRSG, ducting & stack	52,716
Steam turbine , generator & auxiliaries	86,019
Surface condenser	5,986
Feedwater system	16,233
Water makeup & pretreating	2,336
Other feedwater subsystems	4,101
Service water systems	6,996
Other boiler plant systems	8,371
Fuel oil system & nat gas	2,258
Waste water treatment	2,659
Misc. power plant equipment	3,081
Cooling water system	39,714
Accessory electric plant	104,301
Instrumentation & controls	33,030
Improvement to site	23,549
Buildings & structures	22,257
Total	1,761,758
Specific plant cost, $/kW	**3,146**

Table 11. Process Economics – E-Gas and GEP Type Gasifier based IGCC Cases

Gasifier Type	**E-Gas**	**E-Gas**	**GEP**	**GEP**
Cold Gas Cleanup Case	**1**	**2**	**3**	**4**
Basis for Cost Estimates (Year)	2011	2011	2011	2011
Net power, MW	514	553	536	560
Net efficiency, % HHV	30.91	34.45	31.90	34.86
Capacity factor (CF), %	80	80	80	80
Total plant cost (TPC), $	1,767,721,087	1,657,979,242	1,803,840,133	1,761,757,760
6 month labor cost	15,845,106	15,211,860	16,285,705	16,177,408
1 month maintenance materials	2,804,055	2,647,252	2,913,156	2,886,340
1 month non-fuel consumables	846,741	1,153,328	870,082	1,187,439
1 month waste disposal	457,701	449,082	496,036	484,892
25% of 1 month fuel cost at 100% CF	3,043,751	2,934,968	3,074,328	2,940,167
2% of TPC	35,354,422	33,159,585	36,076,803	35,235,155
60 day supply of fuel & consumables at 100% CF	25,686,728	25,433,165	25,974,039	25,541,470
0.5% of TPC (spare parts)	8,838,605	8,289,896	9,019,201	8,808,789
Initial catalyst & chemicals cost, $	16,139,527	17,369,628	16,283,434	18,858,878
Land	900,000	900,000	900,000	900,000
Other owners's costs (15% of TPC)	265,158,163	248,696,886	270,576,020	264,263,664
Financing costs	47,728,469	44,765,440	48,703,684	47,567,460
Total overnight cost, $	2,190,524,356	2,058,990,331	2,235,012,620	2,186,609,422
Fixed operating cost for initial year of operation, $	67,044,634	63,583,305	68,648,213	67,589,971
Annual feed cost at above CF for initial year, $	116,880,029	112,702,790	118,054,204	112,902,405
Other annual variable operating cost at above CF for initial year, $	39,441,574	40,796,747	41,081,034	43,763,244
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year, $	32,314,244	31,074,755	32,268,701	30,750,831
Annual byproduct revenues at above CF for initial year, $	4,228,333	12,064,763	4,270,841	12,230,306
1st year cost of electricity (COE) w/o CO2 TS&M, $/MWh	**136.4**	**119.0**	**133.5**	**123.3**
1st year cost of electricity (COE), $/MWh	**145.4**	**127.1**	**142.1**	**131.1**
1st year CO2 capture cost without CO2 TS&M compared to corresponding IGCC (w/o CO2 capture), $/tonne	42.6	25.9	37.5	28.1
1st year CO2 capture cost without CO2 TS&M compared to SCPC (w/o CO2 capture), $/tonne	61.6	47.3	61.0	53.8
1st year CO2 avoided cost with CO2 TS&M compared to SCPC (w/o CO2 capture), $/tonne	91.2	64.5	85.9	69.9

Table 12. Performance Summary – E-Gas Type Gasifier based F-T Liquids Cases

CASE	5
GASIFIER TYPE	E-Gas
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	130,136
STEAM TURBINE POWER	494,365
TOTAL POWER, kW	624,501
AUXILIARY LOAD SUMMARY, kW	
COAL HANDLING	1,655
COAL GRINDING	8,390
COAL SLURRY PUMPS	2,536
SLAG/ASH HANDLING & DEWATERING	4,130
AIR SEPARATION UNIT AUXILIARIES	4,504
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	147,920
OXYGEN COMPRESSOR	83,691
NITROGEN COMPRESSOR	6,920
SYNGAS RECYCLE COMPRESSOR	5,286
TAIL GAS RECYCLE COMPRESSOR	9,929
CO2 COMPRESSOR	53,997
BOILER FEEDWATER & DEMIN PUMPS	7,289
VACUUM CONDENSATE PUMP	645
PROCESS CONDENSATE & SWS SYSTEMS	702
HUMIDIFIER & BFW CIRCULATING PUMPS	67
COOLING WATER CIRCULATING PUMPS	15,574
COOLING TOWER FANS	7,863
SCRUBBER PUMPS	2,216
RECTISOL UNIT	44,565
GAS TURBINE AUXILIARIES	280
STEAM TURBINE AUXILIARIES	236
CLAUS & TAIL GAS TREATING AUXILIARIES	942
F-T UNIT	70,099
MISCELLANEOUS BALANCE OF PLANT	3,000
TRANSFORMER LOSSES	2,346
TOTAL AUXIIARIES, kW	484,784
NET POWER, kW	139,717
CONDENSER COOLING DUTY	
10^6 kJ/h	2,860
10^6 BTU/h	2,711
F-T LIQUIDS PRODUCTION RATE	
NAPHTHA	
Tonne/D	1,475
ST/D	1,626
DIESEL	
Tonne/D	3,632
ST/D	4,005
CONSUMABLES	
AS-RECEIVED COAL FEED	
KG/h	793,864
lb/h	1,750,470
THERMAL INPUT, KWT HHV	5,987,353
RAW WATER USAGE	
M^3/MIN	49.29
GPM	13,023.49
CARBON CAPTURED, %	91

CASE	6
GASIFIER TYPE	E-Gas
GROSS POWER GENERATED (AT GENERATOR TERMINALS), kW	
GAS TURBINE POWER	130,175
STEAM TURBINE POWER	592,215
TOTAL POWER, kW	722,390
AUXILIARY LOAD SUMMARY, kW	
COAL HANDLING	1,612
COAL GRINDING	8,169
COAL SLURRY PUMPS	2,359
SLAG/ASH HANDLING & DEWATERING	4,054
AIR SEPARATION UNIT AUXILIARIES	4,320
AIR SEPARATION UNIT MAIN AIR COMPRESSOR	148,266
OXYGEN COMPRESSOR	84,199
NITROGEN COMPRESSOR	7,920
SYNGAS RECYCLE COMPRESSOR	5,351
CO2 PURIFICATION & COMPRESSION	90,952
BOILER FEEDWATER & DEMIN PUMPS	9,394
VACUUM CONDENSATE PUMP	574
PROCESS CONDENSATE & SWS SYSTEMS	1,964
BFW CIRCULATING PUMPS	96
COOLING WATER CIRCULATING PUMPS	16,884
COOLING TOWER FANS	8,524
SCRUBBER PUMPS	1,375
DESULFURIZER UNIT	19,788
GAS TURBINE AUXILIARIES	281
STEAM TURBINE AUXILIARIES	258
H2SO4 UNIT	(13,567)
F-T UNIT	60,880
MISCELLANEOUS BALANCE OF PLANT	3,000
TRANSFORMER LOSSES	2,676
TOTAL AUXIIARIES, KWE	469,326
NET POWER, kW	253,064
CONDENSER COOLING DUTY	
10^6 kJ/h	3,185
10^6 BTU/h	3,018
F-T LIQUIDS PRODUCTION RATE	
NAPHTHA	
Tonne/D	1,509
ST/D	1,664
DIESEL	
Tonne/D	3,601
ST/D	3,970
CONSUMABLES	
AS-RECEIVED COAL FEED	
KG/h	793,864
lb/h	1,750,470
THERMAL INPUT, KWT HHV	5,987,353
RAW WATER USAGE	
M^3/MIN	52.14
GPM	13,776
CARBON CAPTURED, %	91

Table 13. Plant Cost Summary – E-Gas Type Gasifier based F-T Liquids Cases

CASE	5
ASU	954,521
Fuel receiving, preparation & feeding	363,954
Gasifier, syngas cooler & auxiliaries	1,136,076
Gasification foundations	76,866
Ash handling systems	148,368
Soot Recovery & SARU	0
Flare stack system	9,280
Shift reactor	3,024
Syngas scrubber (included in gasification auxiliaries)	0
LTGC + Syngas Humidification	92,402
Blowback gas systems	8,840
Fuel gas piping	4,374
Gas cleanup foundations	5,693
Hg Removal	8,727
Rectisol	301,807
Claus & TG Recycle	79,863
CO2 compression, dehydration	108,834
Syngas expander	25,251
Gas turbine, generator & auxiliaries	89,537
HRSG, ducting & stack	25,185
Steam turbine, generator & auxiliaries	104,237
Steam Condensers	11,759
Feedwater system	22,572
Water makeup & pretreating	3,636
Other feedwater subsystems	2,569
Service water systems	23,743
Other boiler plant systems	15,244
Fuel oil system & nat gas	3,113
Waste water treatment	9,024
Misc. power plant equipment	4,409
Cooling water system	91,209
Accessory electric plant	150,163
Instrumentationo & controls	35,775
Improvement to site	55,640
Buildings & structures	44,098
F-T synthesis, product upgrade, PSA & CO2 separation	1,021,624
Total	5,041,418

CASE	6
ASU	967,011
Fuel receiving, preparation & feeding	363,954
Gasifier, syngas cooler & auxiliaries	1,133,159
Gasification foundations	76,738
Ash handling	148,368
Flare stack system	9,280
Warm gas desulfurization	77,874
H2SO4 unit	182,478
Blowback gas systems	8,840
Fuel gas piping	4,404
Gas cleanup foundations	5,737
Trace contaminant removal	13,887
WGS/CO2 PSA	25,924
CO2 purification & heat recovery	4,509
CO2 compression & drying	185,112
Syngas Expander	32,916
Gas turbine, generator & auxiliaries	89,537
HRSG, ducting & stack	25,185
Steam turbine, generator & auxiliaries	118,283
Surface condenser	12,691
Feedwater system	7,428
Water makeup & pretreating	3,784
Other feedwater subsystems	2,920
Service water systems	23,743
Other boiler plant systems	17,392
Fuel oil system & nat gas	3,113
Waste water treatment	9,024
Misc. power plant equipment	4,566
Cooling water system	96,670
Accessory electric plant	160,332
Instrumentationo & controls	35,775
Improvement to site	55,640
Buildings & structures	44,098
F-T synthesis, product upgrade, PSA & CO2 separation	1,044,825
Total	4,995,197

Table 14. Process Economics – E-Gas Type Gasifier based F-T Liquids Cases

Gasifier	**E-Gas**			
Case	**5**		**6**	
Basis for Cost Estimates (Year)	2011		2011	
Chemical-1 (Naphtha), ST/D	1,626		1,664	
Chemical-2 (Diesel), ST/D	4,005		3,970	
Chemical-1 + Chemical-2, ST/D	5,630		5,634	
Chemical-1 RSP/Chemical-2 RSP	0.7742		0.7742	
Net efficiency, % HHV	2.33		4.23	
Capacity factor (CF), %	90		90	
Total plant cost (TPC), $	5,041,417,956		4,995,196,769	
6 month labor cost	51,836,276		50,813,502	
1 month maintenance materials	8,357,671		8,104,413	
1 month non-fuel consumables	2,591,054		3,758,002	
1 month waste disposal	1,771,731		1,640,938	
25% of 1 month fuel cost at 100% CF	10,957,507		10,957,507	
2% of TPC	100,828,359		99,903,935	
60 day supply of fuel & consumables at 100% CF	91,570,355		93,872,280	
0.5% of TPC (spare parts)	25,207,090		24,975,984	
Initial catalyst & chemicals cost, $	18,038,439		59,688,549	
Land	900,000		900,000	
Other owners's costs (15% of TPC)	756,212,693		749,279,515	
Financing costs	136,118,285		134,870,313	
Total overnight cost (TOC), $	6,245,807,417		6,233,961,707	
Fixed operating cost for initial year of operation (OCF), $	204,500,912		201,530,940	
Annual feed cost at above CF for initial year (OCV1), $	473,364,312		473,364,312	
Other annual variable operating cost at above CF for initial year (OCV2), $	137,380,923		145,836,199	
Annual CO2 transporting, storing, and monitoring cost at above CF for initial year (OCV3), $	131,018,834		132,090,919	
Annual byproduct revenues at above CF for initial year (OCV4), $	82,750,720		169,325,339	
	$/ST	**$/bbl**	**$/ST**	**$/bbl**
NAPHTHA				
1st year Required Sale Price (RSP) w/o CO2 TS&M	**938**	**113**	**901**	**108**
1st year Required Sale Price (RSP)	**996**	**120**	**960**	**115**
DIESEL				
1st year Required Sale Price (RSP) w/o CO2 TS&M	**1,211**	**162**	**1,164**	**155**
1st year Required Sale Price (RSP)	**1,287**	**172**	**1,240**	**166**