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Final Technical Report
GTI Project 21510

Low Cost High-H_2 Syngas Production for Power and Liquid Fuels

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DISCLAIMER

ABSTRACT

This report summarizes the technical progress made of the research project entitled "Low Cost High-H_2 Syngas Production for Power and Liquid Fuels," under DOE Contract No. DE-FE-0011958. The period of performance was October 1, 2013 through July 30, 2015.

The overall objectives of this project was to determine the technical and economic feasibility of a systems approach for producing high hydrogen syngas from coal with the potential to reduce significantly the cost of producing power, chemical-grade hydrogen or liquid fuels, with carbon capture to reduce the environmental impact of gasification. The project encompasses several areas of study and the results are summarized here.

(1) Experimental work to determine the technical feasibility of a novel hybrid polymer/metal H_2-membrane to recover pure H_2 from a coal-derived syngas was done. This task was not successful. Membranes were synthesized and show impermeability of any gases at required conditions. The cause of this impermeability was most likely due to the densification of the porous polymer membrane support made from polybenzimidazole (PBI) at test temperatures above 250 °C.

(2) Bench-scale experimental work was performed to extend GTI's current database on the University of California Sulfur Recovery Process-High Pressure (UCSRP-HP) and recently renamed Sulfur Removal and Recovery (SR^2) process for syngas cleanup including removal of sulfur and other trace contaminants, such as, chlorides and ammonia. The SR^2 process tests show >90% H_2S conversion with outlet H_2S concentrations less than 4 ppmv, and 80-90% ammonia and chloride removal with high mass transfer rates.

(3) Techno-economic analyses (TEA) were done for the production of electric power, chemical-grade hydrogen and diesel fuels, from a mixture of coal- plus natural gas-derived syngas using the Aerojet Rocketdyne (AR) Advanced Compact coal gasifier and a natural gas partial oxidation reactor (POX) with SR^2 technology. Due to the unsuccessful experimental results with the hybrid polymer/metal H_2 membrane, a conventional CO_2 capture (single-stage Selexol) and hydrogen purification (PSA) technologies were used in the appropriate cases. In all cases, the integrated system of Advanced Compact coal gasifier, non-catalytic natural gas partial oxidation, and SR^2 multicontaminant removal with state-of-the-art auxiliary system provided a 5-25% cost advantage over the base line plants using GEE coal gasifier with conventional Selexol/Claus sulfur removal and recovery. These plants also produce 18-30% less CO_2 than with the conventional coal gasification plants.

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LIST OF ACRONYMS AND ABBREVIATIONS

AR	Aerojet Rocketdyne (previously PWR) Advanced Compact Gasifier, now GTI R-Gas
ARPA-E	Advanced Research Projects Agency-Energy
ATR	Autothermal Reforming
BACT	Best Available Control Technology
bbl	Barrel
BCP	Breakeven Brent Crude Price
BOP	Balance of Plant
BSD	Barrel per Stream Day (Barrels produced in one 24 hour day)
Btu	British Thermal Units
CAPEX	Capital Expenditures
CB&I	Chicago Bridge and Iron E-Gas Gasifier
Claus	Modified Claus Reaction $2H_2S + SO_2 \rightarrow 3S + 2H_2O$
COS	Carbonyl Sulfide
CTL	Coal To Liquid
C/GTL	Coal and Gas To Liquids
DEG	Diethylene Glycol
DGM	Diethylene Glycol Methylether
DOE	Department of Energy
DoE	Design of experiments
FGD	Flue gas desulfurization
FT	Fischer-Tropsch
GEE	General Electric Energy (former ChevronTexaco) Gasifier
GTI	Gas Technology Institute, a nonprofit, independent research and innovation company
GTL	Gas To Liquids
HHV	Higher Heating Value
HTU	Height of a Transfer Unit = Reactor packing height (feet)/NTU
IGCC	Integrated Gasification Combined Cycle
JSA	Job Safety Analysis
kWhr	kilowatt/hour
L/G	Liquid/Gas
LANL	Los Alamos National Laboratory
lb	pound
LCOE	Levelized Cost of Electricity
LCOH	Levelized Cost of Hydrogen
LHV	Lower Heating Value
Lpm	Liters/minute
M	Thousand
MM	Million
MTG	Methanol to Gasoline process available from ExxonMobil
MW_e	Megawatt electrical
MW_t	Megawatt thermal
NETL	National Engineering Technology Laboratory

Ni	Nickel
NTP	Normal temperature and pressure, 20 °C and pressure of 101 kPa
NTU	Number of Transfer Units (NTU) = $\ln(C_{in}/C_{out})$ where C_{in} and C_{out} are reactor inlet and concentrations of H_2S (or SO_2)
OPEX	Operating Expenditures
PBI	Polybenzimidazole
Pd	Palladium
PEEK	Poly(Ether Ether Ketone)
ppmv	parts per million by volume
POX	Partial Oxidation
PSA	Pressure swing adsorption
RSP	Required Selling Price
PWR	Pratt & Whitney Rocketdyne or Aerojet Rocketdyne, now GTI R-Gas
R&D	Research and development
ROI	Return on investment
RSP	Required selling price
RTI	RTI International is a nonprofit, independent research and innovation company
SCOT	Shell Claus Off-gas Treatment
SCR/SMCR	Selective catalytic reduction and selective non-catalytic reduction processes for NO_x control
SF	Scale factor
SMR	Steam methane reforming
SRNL	Savannah River National Laboratory
SR^2	Sulfur Removal and Recovery, previous UCSRP
SRI	SRI International is a nonprofit, independent research and innovation company
scfh	cubic feet at STP per hour
sccm	Cubic centimeter at NTP
scm	Cubic meter at NTP
STP	Standard temperature and pressure, 68 °F and pressure of 14.696 psia
TEA	Techno-Economic Analysis
TOC	Total Overnight Capital Cost
tpd	Tons (2,000 lb) per day
TPD	Metric Tonne (1,000 kg) per day
TGTU	Tail Gas Treating Unit
TPY	Metric tonne (1,000 kg)/year
TS&M	Transport, Storage and Monitoring of Captured CO_2
UCSRP-HP	University of California Sulfur Removal Process-High Pressure, now SR^2
V	Vanadium
WHB	Waste heat boiler
WGS	Water gas shift $CO + H_2O \Leftrightarrow H_2 + CO_2$

EXECUTIVE SUMMARY

The overall objective of this project was to determine the technical and economic feasibility of a systems approach for producing high hydrogen syngas from coal with the potential to reduce significantly the cost of producing power, chemical-grade hydrogen or liquid fuels, with carbon capture to reduce the environmental impact of gasification. The system of technologies included: 1) coal and natural gas feeding to AR (Aerojet Rocketdyne) Advanced Compact gasifier, 2) GTI's Sulfur Removal and Recovery (SR^2) process for H_2S and multi-contaminant removal, and 3) a novel hybrid polymer/metal membrane for hydrogen separation. GTI has conducted laboratory studies in an attempt to establish the proof-of-concept of a novel metal-polymeric membrane primarily for separating hydrogen and carbon dioxide. In addition, laboratory studies were conducted to obtain additional critical design data for H_2S and multi-contaminant removal using the SR^2 process. These technologies were integrated with the AR gasifier technology and techno-economic analyses performed to determine the benefits of this systematic approach. GTI used coal- and natural gas-derived syngas for power, hydrogen, and liquid fuels and compared the system with current coal technologies.

GTI led the 22-month program, which included research and development (R&D) on:

(1) GTI's novel and patented (US 8,075,671) concept of a "Supported Metal Membrane with Internal Cooling for H_2 Separation". This invention uses a high temperature polymer, such as PBI or porous poly (ether ether ketone) or PEEK, as a porous support in hollow fiber form and uses H_2 permeable metal as the separation layer. The internal cooling fluid keeps the membrane at the desired operating temperature. The internal cooling fluid also acts as a sweep fluid that takes the permeated H_2 out of the hollow fiber. Furthermore, the internal cooling fluid will be pressurized to minimize the pressure differential between the syngas side and the permeate side. After flashing the liquid, nearly pure hydrogen will be produced at a high pressure to feed to the turbine, pipeline, or liquid production plant. Under the current experimental program, GTI was not able to establish the experimental feasibility of the invention.

(2) GTI's Sulfur Removal and Recovery or SR^2 Process integrated with the multi-contaminate removal process for sulfur and trace components removal from syngas. DOE has supported the development of this syngas gas cleanup technology in the laboratory and bench-scale that has treated syngas to <30 ppm H_2S at ~175 °C with up to 6,000 ppm H_2S in the feed. The SR^2 technology relies on a liquid phase Claus reaction of H_2S with SO_2 to convert H_2S to molten sulfur and water. Unlike the conventional gas phase Claus process, the SR^2 process is not equilibrium limited and can reach very low H_2S concentrations in the treated syngas. Testing in this study was focused on collecting kinetic data for the removal of low levels (<50 ppmv feed) of H_2S, and trace component (primarily chlorides and ammonia) removal in the co-current down-flow contactor.

(3) Using data from these R&D efforts, we conducted conceptual designs and techno-economic analysis (TEA) to estimate plant efficiency, product costs, and environmental performance for three base-case process configurations involving the Advanced Compact Coal Gasifier and natural gas partial oxidation reactor and the SR^2 technologies for: IGCC plant, chemical-grade hydrogen, and production of liquid fuels, primarily diesel using a Fischer-Tropsch technology. Syngases are generated via

gasification of Illinois #6 coal and partial oxidation of natural gas with the coal contributing >50% of the total caloric value in the plant. All designs achieved at least 90% carbon capture. Due to the unsuccessful R&D results on the hybrid membrane, conventional technologies were used for carbon capture (single-stage Selexol) and hydrogen purification (pressure swing adsorption {PSA}) as appropriate in these studies.

Potential impact of project benefits and outcomes:

- AR gasification technology: Best-in-class gasification process for power and hydrogen production with conventional technologies with about 13-25% lower cost than conventional technology. For the proposed economic evaluation, the use of AR gasification technology is to lead to about 90% reduction in the gasifier volume, 50% reduction in the capital cost of the gasification system, and over 99% carbon conversion.[2]
- POX technology: Operates at very low steam to carbon ratios without forming coke resulting in lower oxygen requirements. Natural gas POX operates at a much higher outlet temperature than achievable with coal gasification. This allows for significant heat recovery via waste heat boiler (WHB) and hence greater electricity production.
- Near-zero emissions of H_2S and trace contaminants from the integrated process due to integrating SR^2 process for H_2S/trace-components removed.
- Compact and simple equipment: Process intensification with compact gasifier/POX and integrated processes. No moving/circulating solids at high pressures in the syngas treating system.
- Flexibility and Efficiency: Plant systems can be optimized for power, chemical hydrogen, or liquid fuels and large temperature swings are minimized.
- Lower cost: Capital and operating costs are projected to be lower for hydrogen, electricity, and liquid fuel.
- Lower environmental impact: 18-30% less CO_2 is produced that requires sequestration.

AR provided energy and material balances for their gasifier with coal and POX with natural gas in addition to experimental data obtained by GTI to produce a high hydrogen syngas. These data were used in the economic study to establish an optimum natural gas to coal ratio between zero and 50% by heating value. GTI had tried to determine the technical feasibility of a novel hybrid metal/polymer membrane by alloy deposition on surface of hydrogen-selective, temperature-resistant polymer polybenzimidazole (PBI) membrane substrate to produce a hydrogen membrane with near infinite selectivity. SRI provided flat sheets of PBI substrate with various pore sizes and porosities for metal coating by GTI. The pore sizes were found to be inconsistent. Thin layers of metal/alloy were deposited on porous polymer support using "magnetron sputtering". GTI tested the membranes (metal-coated substrates) using hydrogen and helium gases for hydrogen permeation and selectivity. When the metal layers were not dense enough to completely block the pores in the substrate, both gases would flow through the membrane with essentially no selectivity. The testing of synthesized membranes with sufficient density to prevent helium transport showed a complete impermeability for hydrogen as well due to either densification of the porous PBI support at the temperatures required for hydrogen permeation or vanadium oxide layer formation.

GTI conducted laboratory experiments on SR^2, an integrated multi-component removal process. Studies were conducted in a co-current reactor to determine the design conditions necessary to achieve low levels of H_2S in the treated syngas and to maximize the removal of impurities (HCl and NH_3). More than 95% H_2S conversion for 2nd stage reactor was obtained. The extent of the removal of trace amounts of chlorides and ammonia using three solvents: DGM, DEG, and water, were investigated. More than 80% HCl removal was obtained for all three solvents (DEG, DGM and water). NH_3 removal was more than 80% with water, but less than 75% with DEG or DGM. Water was chosen as solvent of choice for the trace contaminant removal in the co-current contactor.

GTI planned to perform conceptual designs and TEA to estimate plant efficiency, cost of products, and environmental performance for three Base-Case configurations, Integrated Gasification Combined Cycle (IGCC), chemical-grade hydrogen, and diesel, involving integrations of the hydrogen membrane and the SR^2 technologies into AR gasification system where appropriate, all with carbon capture. Since an acceptable membrane was not identified, a single-stage Selexol unit was used for CO_2 capture in the IGCC and hydrogen cases and a PSA unit was used to produce the 99.9% pure product in the hydrogen study. The design and economics of GTI's multi-contaminant removal process was previously published [4]. Summary of key results and conclusions are given in the Table 1.

The TEA of the Integrated Gasification Combined Cycle (IGCC) case addresses the production of power, via the integration of AR coal gasifier and a natural gas partial oxidation reactor with GTI's SR^2 integrated multi-contaminant removal process. The performance and economics are compared to a study performed by DOE-NETL on GEE gasification facility [3] for power production, namely case B5B-Q. The GTI process, with 51% of the input energy coming from coal, showed 20% savings in CAPEX and OPEX resulting in a reduction in levelized cost of electricity (LCOE).

The TEA addresses the production of chemical grade H_2, via the integration of AR coal gasifier and a natural gas partial oxidation reactor with GTI's SR^2 with integrated, multi-contaminant removal process, and a PSA unit. This case compared the AR Advanced Compact Gasifier and POX with the GEE gasifier in hydrogen production and carbon capture mode [DOE/NETL-2010/1397] [5]. Chemical-grade hydrogen production was studied with 51% of the plant energy input coming from coal and 49% coming from natural gas being partial oxidized to syngas. When compared at the same plant size, GTI's hydrogen plant would be able to produce hydrogen at about 20% lower cost than in the DOE CTL case.

In the diesel production study, the TEA addresses the production of liquid fuels, namely Fischer-Tropsch (FT) liquids, via the integration of AR coal gasifier and a natural gas partial oxidation reactor with GTI's SR^2 with integrated multi-contaminant removal process and the FT conversion process. The performance and economics are compared to a study performed by DOE on small-scale CTL plants in West Virginia, namely Concept 2 in DOE/NETL 2007/1253 [1]. In that study, two 300 MW_e GE gasifier trains, produce syngas that is converted into 9,609 bbl/day of diesel and naphtha using FT technology. GTI's C/GTL Production case showed 25% savings in CAPEX and OPEX as compared with DOE CTL base case when 53% of the energy input was from coal.

Comparing the amount of CO_2 captured that requires sequestration, the GTI conceptual plants produced 30% less for the liquids production plant and 18% less for the hydrogen and

IGCC plants than the similar sized, coal-only plants.

The composite metal/high-temperature polymer hollow fiber membrane concept, if developed, could have the potential to substantially increase the packing efficiency of earlier proposed metal hydrogen separation membranes and further reduce the cost and size of the separation system for these applications over potential membranes that meet DOE’s 2015 Performance Targets [6].

Table 1 Key Comparative Basis and Data

Subtask	**4.1**		**4.2**		**4.3**	
Case	**DOE Base IGCC**	**GTI IGCC**	**DOE Base Hydrogen**	**GTI Hydrogen**	**DOE Base CTL**	**GTI C/GTL**
DOE design reference	DOE/NETL-2015/1727 Case B5B-Q	DOE/NETL - 401/062006 Case 1	DOE/NETL - 2010/1434 Case 2-2	DOE/NETL - 401/062006 Case 5	DOE/NETL - 2007/1253 Concept 2	DOE/NETL - 401/062006 Case 1
Coal gasifier technology	GEE Quench	AR	GEE Quench	AR	GEE Quench	AR
Natural gas to syngas technology	--	POX	--	POX	--	POX
H_2S separation/ sulfur recovery	Selexol 1st stage /Claus /hydrogenation recycle	SR^2	Selexol 1st stage /Claus /hydrogenation recycle	SR^2	Selexol single stage /Claus /hydrogenation recycle	SR^2
CO_2 capture	Selexol 2nd stage	Selexol one stage	Selexol 2nd stage	Selexol one stage	Amine one stage	Selexol one stage
Product preparation	--	--	PSA H_2 purification	PSA H_2 purification	Iron-based FT catalyst	Iron-based FT catalyst
Plant size	492MW_e	514MW_e	619 TPD H_2	668 TPD H_2	9,609 BSD FT liquids	9,610 BSD FT liquids
Coal feed rate (as received), TPD	5,301	2,634	5,301	2,634	3,859	1,961
Natural gas feed rate, TPD	--	1,393	--	1,393	--	981
Input energy from coal, %	100	51	100	51	100	53
O_2 Needed, TPD	4,343	4,280	4,324	4,280	3,565	3,313
Total CO_2 sequestered, TPD	10,951	8,957	10,958	8,957	4,807	3,411
Power generation, MW_e	684	682	113	117	113	144
Total auxiliary load, MW_e	191	168	148	131	80	71
Import (export) electricity, MW_e	(492)	(514)	35	14	(33)	(73)
CAPEX, $MM	1,630	1,291	1,411	973	927	660
Annual Fuel cost, $MM/yr	68	114	76	129	57	90
Product cost w/TS&M	$134/$MW_e$	$127/$MW_e$	$3.41/kg H_2	$2.71.kg H_2	$63/bbl BCP	$47/bbl BCP

OBJECTIVES AND INTRODUCTION

Objectives

The main objective of this project is to determine the technical and economic feasibility of a systems approach for producing high hydrogen syngas from coal that has the potential to reduce significantly the cost of producing power, chemical-grade hydrogen or liquid fuels, with carbon capture to reduce the environmental impact of gasification. The technology is an integrated scheme that includes coal and natural gas feeding to an AR gasifier and a POX reactor, respectively, GTI's SR^2 process for H_2S and multi-contaminant removal and a novel hybrid polymer/metal membrane for hydrogen separation. GTI economic studies for the SR^2 process have shown significant economic incentives in developing an advanced H_2 membrane for IGCC with carbon capture.[4] The use of AR gasification technology may lead to ~90% reduction in the gasifier volume, 50% reduction in the capital cost of the gasification system and over 99% carbon conversion.[2]

Task 1 of the project "Project Management, Planning and Reporting" was to manage and direct the project in accordance with the agreed to Project Management Plan (PMP) to meet all technical, schedule and budget objectives and requirements.

Task 2 of the project "Development of Novel Hydrogen/Carbon Dioxide Separation Membranes" was to synthesize novel hybrid metal/polymer membranes by alloy deposition on surface of hydrogen-selective flat sheet polymer support to prepare hydrogen membranes with high hydrogen selectivity. The promising membranes were tested using binary and simulated syngas mixtures for hydrogen permeation and selectivity. The best membrane identified from permeation tests was to be the basis of the techno-economic analysis.

Task 3 of the project "Extended Design Data of an Integrated Multi-Component Syngas Impurity Removal Process" was to study the UCSRP-HP or SR^2 process at bench scale with different inlet H_2S and SO_2 concentrations with a target of less than 4 parts per million by volume (ppmv) H_2S on the reactor outlet. Other tests will be done to determine the removal efficiency of the reactor packed with Sulzer SMV^{TM} static mixer for trace components.

Task 4 of the project "Conceptual Design and Techno-Economic Evaluation of Low Cost High-H_2 Syngas Production System" was to conduct preliminary conceptual designs and techno-economic analyses to estimate plant efficiency, cost of products, and environmental performance for three base-case configurations involving integrations of the novel hydrogen membrane and the UCSRP-HP technologies where appropriate into an AR gasification system, all with carbon capture.

Introduction

New markets can be found with the development of cost-effective technologies for hydrogen production in the power and liquids markets. Gasification systems can operate with less environmental impact and at lower costs than alternative systems. However, to be able to produce hydrogen for power, chemicals or clean fuels, the hydrogen content of the coal-derived syngas must be increased from H_2/CO ratios of ~1 from commercial gasifiers to ~1.8-2.1 as needed for Fischer-Tropsch diesel or MTG (methanol-to-gasoline) gasoline production, or to "pure" H_2. Under this project, to reduce the extent of carbon capture requirements for a given plant capacity, TEA was performed for gasification of coal and natural gas (with coal contributing at least 51% of the total caloric value of the plant feed) in an AR compact gasifier that uses dry coal feed and a POX reactor.

SR^2 and metal/polymer composite hydrogen membrane technologies were planned to be integrated with other commercially available processes for the production of electric power, chemical-grade hydrogen or clean fuels from coal/natural gas derived syngas gas with carbon capture.

Certain alloys involving palladium (Pd) or group of refractory metals are highly permeable and perfectly selective for hydrogen separation from other gases. Vanadium (V) alloys have an order of magnitude higher permeability than that of Pd alloys in the temperature range under consideration and are easier to fabricate than other high permeability refractory metals. However, they are prone to oxidation and relatively poor at catalyzing H_2 surface reactions. The GTI membrane concept involves Pd-coating onto both sides of a dense, thin, V-alloy layer which is supported by hollow fibers. The Pd outer layers catalyze H_2 dissociation and recombination reactions and protects alloy from oxidation. The alloying of vanadium may prevent hydrogen-embrittlement problems.

Various R&D groups have explored the potential of specific metal-alloy membranes due to their 100% selectivity and relatively high permeability for hydrogen in gas purification and reactor applications. These studies have focused primarily on key Pd alloys such as Pd-Ag, Pd-Au, and Pd-Cu because of their ability to catalyze hydrogen surface reactions, permeate atomic hydrogen, resist oxidation, and avoid hydrogen embrittlement. However, these efforts have led only to niche applications and have not met the rigorous requirements for large-scale industrial processes such as coal gasification. A few other important research efforts have been conducted using coated V-alloy membranes at organizations such as Eltron, REB Research, LANL, NETL, and SRNL.

GTI's novel membrane technology (see Figure 1) has the potential to exceed the performance characteristics of currently developing H_2 membranes due to the following reasons:

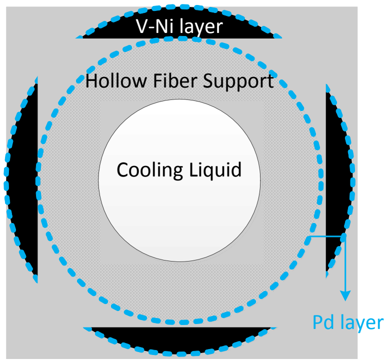


Figure 1 A Schematic of the Proposed Hybrid Hydrogen Membrane

a. Thinner metal/alloy layers require less material and membrane should have a higher hydrogen flux due to reverse proportionality of flux and thickness.

b. GTI's hydrogen membrane uses a liquid for sweeping hydrogen. The liquid, therefore, plays several roles; it cools down the membrane to have more thermal stability for polymer support, it minimizes the trans-membrane pressure, it allows the recovery of hydrogen at pressure, and it carries hydrogen from the permeate surface. Factors such as the ease of separation of hydrogen from the cooling liquid, and the ability to maintain low hydrogen partial pressure in the permeate side even after cooling fluid compression by regulating the liquid flow rate, add to the overall cost effectiveness of the technology.

c. Counter-current flow of syngas and cooling liquid with hydrogen results in higher efficiency for hydrogen separation.

d. Hollow fiber membranes have high area/volume ratio reducing the size and weight of the high-pressure vessel shells and helping to make the process more economically viable. Further, the hollow fiber-based membranes are easily scaled-up.

On a long-term basis of coal gasification development, there is still the need for low-cost sulfur removal technologies for reducing the net cost of electricity in IGCC applications if and when CO_2 removal and sequestration are necessary for new coal-based power plants. Currently, low temperature absorption processes such as Rectisol™ or Selexol™ are employed to scrub the gas and remove the sulfur compounds. The SR^2 technology seems to be an economically attractive concept for sulfur removal in coal/coke gasification, and in natural gas or oil-shale processing applications. Previously, in a Gas Research Institute sponsored techno-economic evaluation of the low pressure UCSRP process conduction by KBR Halliburton, KBR had found significant advantages of the UCSRP with 40% reduction in capital and operating cost for this technology as compared with conventional treating approaches, i.e., Claus plus Shell Claus Off-gas Treatment (SCOT) tail gas treating unit (TGTU). Testing done at GTI has shown negligible chemical consumption (including catalyst), unlike typical chemical costs of \$300-\$1000 per ton sulfur removed found in competing processes. The process can operate at significantly higher temperatures than the liquid redox or CrystaSulf processes, which is of value in IGCC applications.

For this project, we obtained experimental kinetic data for the key sulfur formation reaction under specific SR^2 operating conditions and for the removal of impurities, such as ammonia and chlorides. These results helped in the design of down-flow co-current type commercial reactors and expanded our knowledge base to build a pilot-scale facility for verifying the overall integrated SR^2 process. Further improvements of the gasification technology studied in this project may significantly enhance the acceptance of coal as a feedstock. The ability to reduce the cost for sulfur and other coal impurities may lead to a greater usage of the high-sulfur coals that are not currently competitive for power generation.

GTI's initial concepts in the integration of the H_2 membrane along with the SR^2 process for commercial IGCC and liquid-fuel applications are shown schematically in Figure 2 and Figure 3. Note the schemes have co-feeding of coal and natural gas to the AR gasifier. Co-gasification leads to a syngas with relatively higher H_2/CO level compared to the gasification of coal alone. For the co-gasification of coal/natural gas, about 51% of the energy in the feed is derived from coal (e.g., coal at 3,000 T/day and natural gas at 1,800 T/day). The H_2/CO molar ratio from gasification of coal only would be ~0.5 vs. ~1.8 for natural gas. Thus, for the co-gasification case, the effluent syngas would have a H_2/CO ratio of ~1.1. Shifting about 35% of the sweet syngas and separating the CO_2 brings the H_2/CO molar ratio of feed to the liquids plant to approximately two.

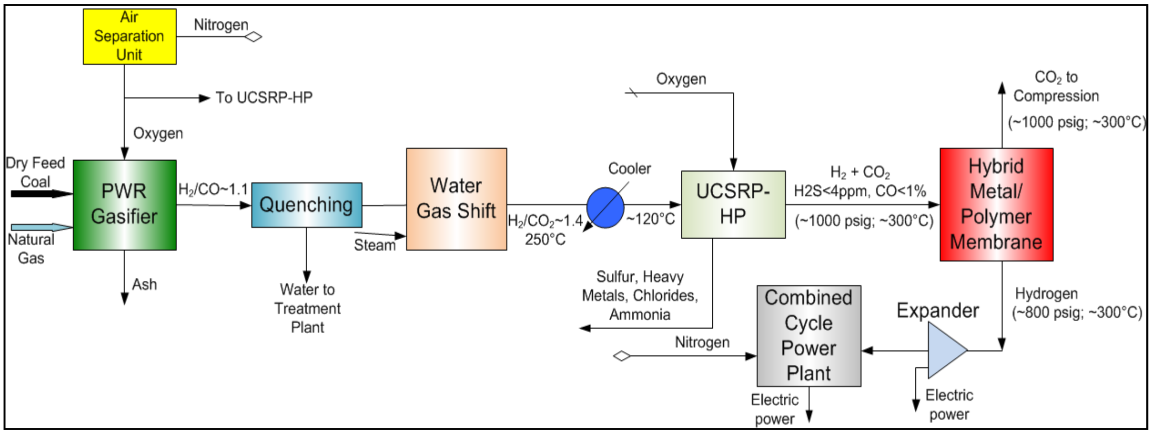


Figure 2 Conceptual Flow Sheet for Option 1: Coal/Natural Gas-based IGCC or Chemical-grade Hydrogen with Carbon Capture

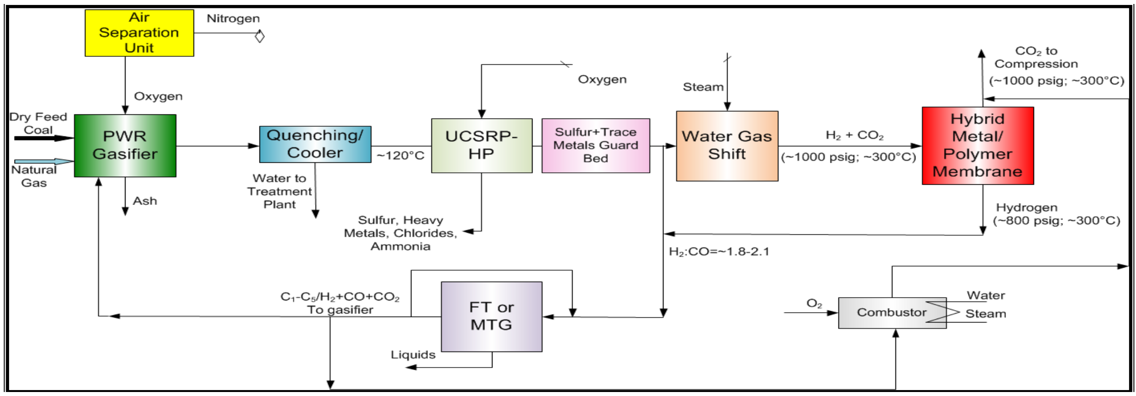


Figure 3 Conceptual Flowsheet for Option 2: Coal/Natural Gas-based Liquid Fuels Production with Carbon Capture

In this part of the study, we planned to conduct conceptual designs and TEA to estimate plant efficiency, product costs, and environmental performance for three base-case process configurations involving integrations of the novel H_2-membrane and the SR^2 technologies with the coal/natural gas fed AR gasifier: (1) IGCC plant with carbon capture (>90% based on the raw syngas carbon content) with power generation of ~464 MW_e from H_2-rich gas using two advanced GE F-class turbines, (2) chemical-grade hydrogen with carbon capture and (3) production of ~50,000 barrels/day of liquids fuels, primarily diesel, using a FT technology with carbon capture (~87% carbon capture based on the raw syngas carbon content). Syngas were generated via gasification of a mixture of Illinois #6 coal and natural gas, with the coal contributing >50% of the total caloric value in the feed, in a AR compact gasifier using dry coal feed to reduce oxygen consumption.

EXPERIMENTAL PROCEDURES

Task 2: Development of Novel Hydrogen/Carbon Dioxide Separation Membranes

Subtask 2.1 – Preparation of Polymer Substrate

For the proposed exploratory development program, we proposed to show the technical feasibility of the separation using SRI-provided flat sheets of PBI rather than hollow fibers. SRI used its membrane fabrication process and employed new cross-linking procedures to prepare the flat sheet membranes. The aprotic non-solvent acetonitrile has also been employed that allows facile removal of cast membranes from the glass casting substrate in less than 30 sec, permitting better control of membrane uniformity. SRI's standard membrane annealing process is carried out in the presence of ethylene glycol that is sometimes trapped in the film. SRI have modified the annealing process by achieving chemical cross-linking using 1,4-dibromobutane in methyl isobutyl ketone at 100 °C and subsequently drying the samples above 150 °C for a few hours.

Subtask 2.2 – Synthesis of Hydrogen Selective Membranes

The proposed membrane uses a high temperature polymer, such as PBI, as a porous support in flat form and a specific H_2-permeable metal-matrix (Pd/V-Ni alloy/Pd) as the separation layer.

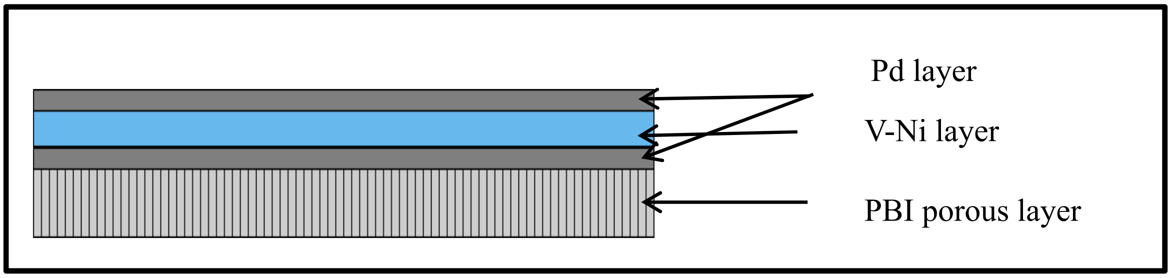


Figure 4 GTI's Conceptual Hydrogen Membrane

In this subtask, GTI deposited metals on PBI substrate-see Figure 4. The synthesis consisted from the following steps: (1) Deposition of palladium on porous support by sputtering. Thickness was varied from 0.05 to 1 microns; (2) Sputtering of V-Ni alloy on Pd-polymer surface. Deposited V-Ni alloy layer carried from 1 to 3 microns in thickness; (3) Deposition of palladium on porous support by sputtering. Thickness was varied from 0.05 to 1 micron as in first step. The thickness of layers was varied based on permeability data. Also ion sputtering was used to deposit denser metal films.

Subtask 2.3 – Testing Hybrid Metal/Polymer Membrane for Hydrogen Permeation Performance

The objective of this subtask was to collect hydrogen permeation data in the membrane unit under a controlled laboratory environment for the membranes selected and fabricated in Task 2. Membrane sealing issues were resolved during this task. Initial tests were performed using H_2 and He gases to obtain hydrogen permeability data. Membrane testing was conducted in a permeation cell (Figure 5) at temperatures up to 250 ºC and pressures up to 13 atm. A permeation cell was constructed for testing hydrogen permeation and selectivity at the targeted temperature of 250°C. Membranes were sealed using O-rings and compression fitting in the test cell. This cell allows screening and testing of candidate membrane materials. Porous stainless steel supports (pore size 20 microns) was positioned in a recess. The membrane was placed on top of the porous stainless steel support and the O-rings (Viton, high-temperature Teflon) were used as a seal. All testing was done with flat membrane disks as proposed to prove the concept. If successful, the membranes would be further developed into hollow fibers.

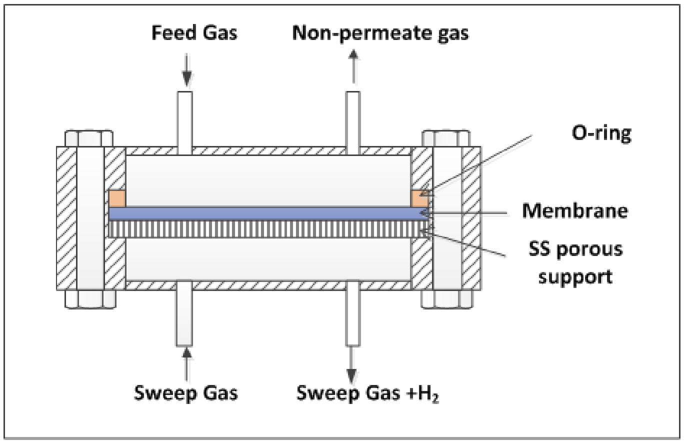


Figure 5 Scheme of Membrane Test Cell

The permeation unit process and flow diagram is shown in Figure 6. Pure component from the gas feeding system flows on top of the membrane and the permeate gas is collected on the bottom of the membrane for flow measurement and gas analysis. Permeation fluxes were calculated using bubble meter. The unit allows membrane permeation testing with different gases and was used to evaluate porous supports for pore size and permeance. When a porous support material was identified to have the required permeance and selectivity performance, metal layers were deposited on it and testing of hydrogen and helium permeation flux and selectivity were performed under the required temperature and pressure conditions.

Task 3.0 –Extended Design Data of an Integrated Multi-Component Syngas Impurity Removal Process

Subtask 3.1 – Testing the UCSRP-HP Process for Low-level Sulfur Removal

Under this subtask, we used the existing bench-scale down-flow co-current sulfur-removal reactor fitted with Sulzer SMV^{TM} packing to study the extent of H_2S removal with low levels (~30-500 ppmv) of inlet H_2S. The key objective was to identify operating conditions to have a H_2S level of <4 ppmv in the reactor exit gas. The levels of SO_2 in the primarily nitrogen feed gas were to be maintained at about 1-10% excess over that needed for the stoichiometric Claus reaction: $2H_2S + SO_2 = 3S + 2H_2O$

The operating pressure for the testing was ~100-400 psig with a nominal inlet feed gas temperature of ~120 ºC. The solvent/feed gas mass ratio was varied.

Subtask 3.2 – Testing the UCSRP-HP Process for Trace Component Removal

The same down-flow co-current bench-scale reactor, fitted with a SMV packing unit, was modified to explore the extents of the removal of trace amounts of chlorides and ammonia using three solvents: DGM, DEG, and water. Water was shown to be the best solvent at a nominal gas flow of 2 ft/s and it was further tested at different L/G mass ratios in the ~0.5-3.0 range for chlorides and ammonia removal. The bench-scale unit consists (see Figure 7) of a down-flow co-current reactor packed with a 3-ft-long section of SMV^{TM} static mixer and placed in an oven to maintain an inlet reactor temperature above 245 °F to prevent sulfur condensation and plugging. Four mass flow controllers deliver nitrogen, sulfur dioxide, carbon dioxide and hydrogen sulfide gases. A 4-in.-diameter tank/3-phase tank separated gas and liquids, including sulfur, after the gas exits the reactor. A solvent pump was used to re-circulate the different solvents. A 9 kW Chromalox® heater maintained the re-circulating solvent at the desired process temperature.

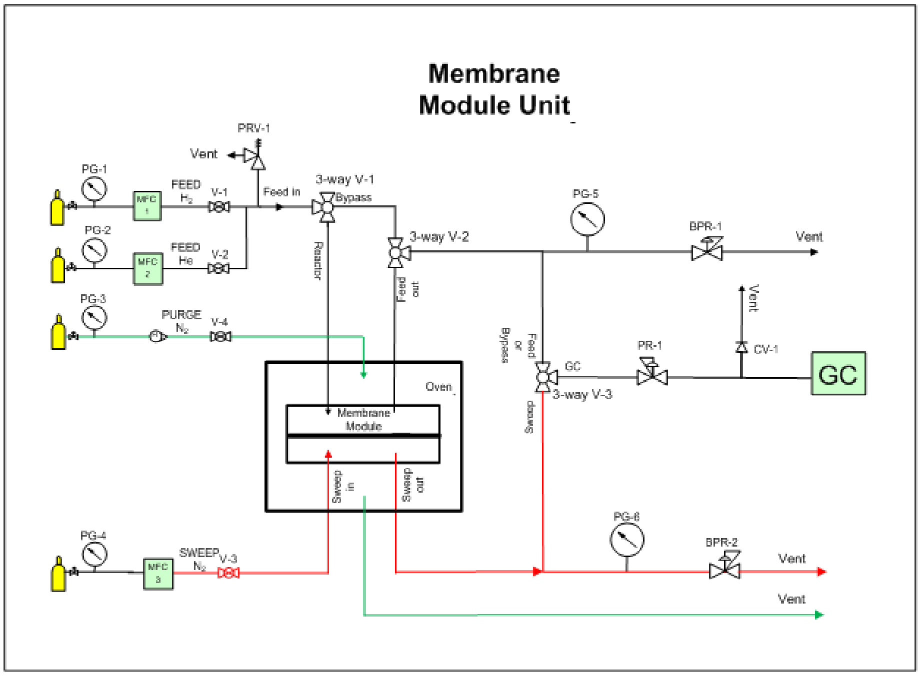


Figure 6 Membrane Permeation Test System Flow and Instrument Diagram

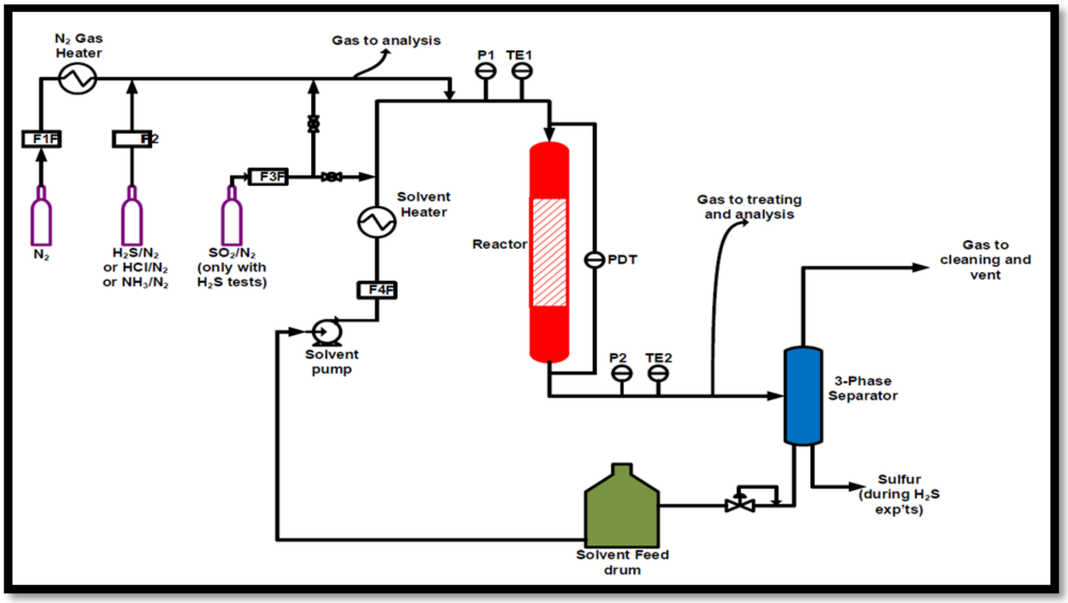


Figure 7 Simplified Schematic of the GTI's Bench-scale SR^2 Reactor System

RESULTS AND DISCUSSION

Task 2: Development of Novel Hydrogen/Carbon Dioxide Separation Membranes

Subtask 2.1 – Preparation of Polymer Substrate

In this subtask, SRI was contracted to synthesize porous flat membranes from the temperature-resistant polymer PBI and provided GTI with 46 different PBI supports in total. The target flux for hydrogen membrane in our project is 100 scfh/ft^2 at a hydrogen partial pressure difference of 100 psi, which equals to 50.8 cm^3(STP)/(min•cm^2). All tested substrates were compared to the target value. Based on past results a target value for helium permeation was calculated and should be in range 10-80 cm^3/min-cm^2 at 25 ºC and pressure difference 100 psi to have target hydrogen flux. Table 2 shows the results of pure He or pure H_2 diffusion flow at various temperatures and pressures through the porous substrates made by SRI.

From the batch of porous substrates, substrates: #15B-1, #16B and #20 (in Table 2 substrates 15B-1 and 16B start with SB initials) were chosen. Table 3 shows reproducibility results for chosen substrates for pure gas components. Helium permeation testing was done at room temperature and pressure difference of 100 psi. Based on consistency of results and reproducibility in manufacture, substrates #16B and # 20 were chosen as a final selection.

Subtask 2.2 – Synthesis of Hydrogen Selective Membranes

Due to possible thermal stress which may occur during sputtering process, two substrates of each sample #16 and #20 were thermally treated before metal deposition. The samples were placed between glass sheets and heated to 250 ºC in air for 10 hours. Then four substrates (2 of each substrate and 2 of them thermally treated) were sent to Intlvac Thin Film for metal deposition. The substrates were mounted on thermally conductive gasket material and supported by a chrome plated copper platen rotating at 30 rpm. The substrates were pre-cleaned with Argon ions and then a three-layer metal was deposited on the PBI substrate. The metal layer consisting of 1µm Pd, 3µm Ni-V, and 1µm Pd was deposited via DC sputter at low power. The chamber was slowly vented to atmospheric pressure using dry nitrogen upon completion of the coating. Post run profilometry measurements show overall thickness of 5.8 µm while the target thickness was 5 µm. Overall metal adhesion to the substrate was good. After frame removal, due to stress of support and deposited metal, the substrates as shown on Figure 8 became curled and integrity of supports was destroyed.

After sputtering process, membranes were subjected to heating (temperature equals 125 ºC) for 2 hours to reduce tensile and compressive stress and uncurl samples. Membranes after the treatment were essentially free of stress and were tested for helium and hydrogen permeation.

Based on the permeation results shown in next paragraph, parameters for the sputtering process were changed to deposit a more dense metal coating on substrates. In addition, ion source was used for membrane synthesis to produce more dense films. Four more membranes were synthesized using: two sheets of #16 (with and without ion source) and two of # 20 samples (with and without ion source). Thickness of layers in the case of ion source assistance was 0.5 µm Pd, 1 µm Ni-V, and 0.5 µm Pd. Two other membranes have the same thickness for Pd layer, but 2 µm Ni-V layer.

Table 2 Permeation Properties of Porous Substrates Developed by SRI

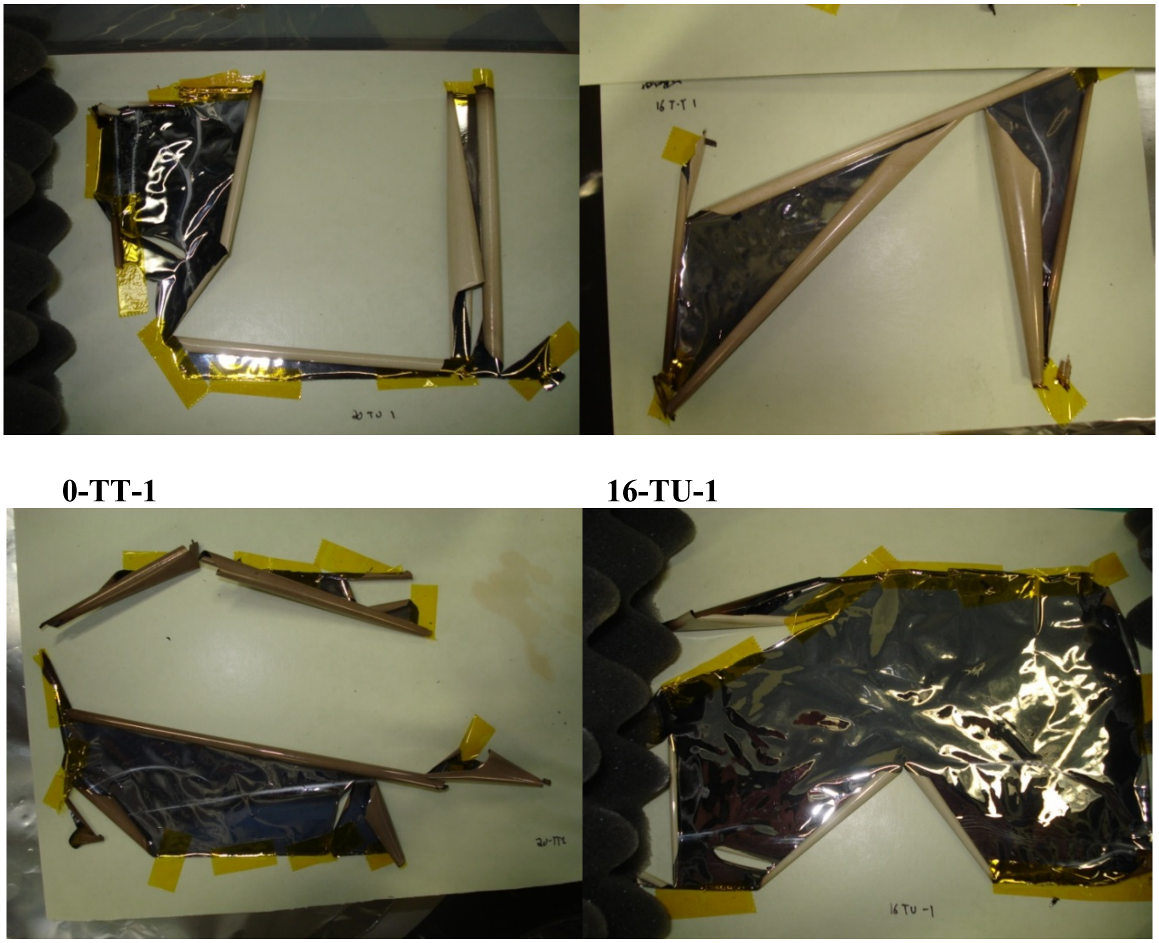
SRI Substrate	**T, ºC**	**Delta P, psi**	**H_2 Permeate flux, cm^3/min-cm^2**
14I-C/1	100	400	0
14I-C/2	250	400	2
14I-NC	25	400	0*
14M-C/1	250	400	44
14M-C/2	250	400	355
14M-C/3	250	400	257
14M-C/4	250	100	8
14M-NC	250	80	378
32014-I	25	400	0*
32014-MD	250	100	42
32015-I/1	25	110	0*
32015-I/2	25	110	0*
32015-I2/1	16	400	0*
32015-I2/2	16	400	0*
32015-I3/1	16	400	0*
32015-I3/2	16	400	0*
32015-MD	250	100	39
7A/1	25	10	194*
7A/2	25	10	194*
7B	250	100	59
7B after 15 hours at 250ºC in He	250	100	38
9A	25	400	0*
9B	25	400	8*
9C	25	400	0*
9D	25	400	15*
9E	250	100	51
9E after 15 hours at 250ºC in He	250	100	42
9F	250	100	78
9F after 22 hours at 250ºC in He	250	100	60
SB-5A	25	400	0*
SB-6A	25	300	0*
SB-7A	25	100	13*
SB-8A	25	400	0*
SB-9A	25	400	0*
SB-10A	25	400	0*
SB-11A	25	400	0*
SB-3B	25	400	0*
SB-5B	25	400	0*

SB-6B	25	400	0*
SB-7B	25	100	0*
SB-8B	25	100	0*
SB-9B	25	100	0*
SB-11B/1	25	60	189*
SB-11B/2	25	40	187*
SB-12B	25	100	0*
SB-13B	25	400	9*
SB-14-1B	25	100	9*
SB-14-2B	25	400	0*
SB-14-3B	25	400	0*
SB-14-4B	25	400	0*
SB-15B-1B/1	250	100	131
SB-15B-1B/2	25	100	0*
SB-15B-1B/3	250	100	59
SB-15B-1B/3 after 20 hours at 250ºC in helium	250	100	83
SB-15B-2B	25	400	6*
SB-15B-3B	25	400	0*
SB-15B-4B	25	400	0*
SB-16B/1	250	100	122
SB-16B/2	250	100	179
SB-16B/2 after 15 hours at 250ºC in helium	250	100	145
SB-17B	25	100	105*
20/1	16	100	20*
20/2	16	20	197*
20/3	16	100	20*
20/3	250	100	138

*- Helium permeation values. Due to very low helium permeation flux, no test for hydrogen permeation was done.

Table 3 Reproducibility Testing of Manufacture of Chosen Substrates: 15B-1 and 16B

Substrate	Sheet#-sample#	T, ºC	Δ P, psig	He Permeate flux, cm^3/min-cm^2
15B	1-1R	15	100	7
15B	1-2R	15	100	0
15B	1-3R	15	100	89
15B	2-1R	15	100	141
15B	2-2R	15	100	60
15B	2-3R	15	30	194
15B	3-1R	15	100	13
15B	3-2R	15	100	108
15B	4-1R	15	100	0
15B	4-2R	15	60	194
15B-LV	1	16	100	11
15B-HV	1-1	16	100	2
15B-HV	2-1	16	100	65
15B-HV	2-2	16	100	7
16B	1-1R	15	30	196
16B	1-2R	15	100	169
16B	2-1R	15	30	196
16B	2-2R	15	40	193
16B	3-1R	15	30	196
16B	3-2R	15	40	196
16B	4-1R	15	40	196
16B	4-2R	15	100	45
16B	4-2R	15	100	48
16B	3-2R	15	100	145
16B	3-3R	15	40	193
16B-LV	1	16	50	197
16B-HV	1-1	16	30	197
16B-HV	2-1	16	30	197
16B-1	1	16	20	197
16B-2	1	16	20	197
20-1	1	17	100	15
20-2	1	17	100	7
20-R	1	17	100	10
20-R	1	250	100	194
20-R	2	20	100	10
20-R	2	250	100	182


20-TU-1 **16-TT-1**

0-TT-1 **16-TU-1**

Figure 8 Membranes after Sputtering

The substrates were mounted on thermally conductive gasket material and supported by an aluminum frame mounted on a chrome plated copper platen rotating at 30rpm. The substrates were pre-cleaned with krypton ions and then 0.5 µm Pd, 1 µm Ni-V, and 0.5 µm Pd was deposited via DC sputter at high power with a krypton ion assist. A second run was repeated without ion assist while depositing 2.0 µm of Ni-V instead of 1 µm. The chamber was slowly vented to atmospheric pressure using dry nitrogen upon completion of the coating. Post run profilometry measurements show overall thickness for the first run of 2.1 µm and for the second of 3.06 µm while the target thickness was 2 µm and 3 µm respectively. Overall, metal adhesion to the substrate was good. Due to stress phenomena, synthesized membranes were packaged using low-lint paper inside heavy cardstock and heavy foil to avoid repeating of the rolled edging. Still the thermal treatment was needed- heating at 125 ºC for two hours has reduced the film stress. The samples were flattened and tested for hydrogen and helium permeability.

We have also tested a ceramic support instead of the PBI supports to verify the hypothesis of support densification. Ceramic supports are expected to be stable at high temperatures; therefore we do not anticipate any blocking of pores when operating at 300 or 350 °C. We had previously purchased ceramic supports from Cobra Technologies with a pore size of 80 nm and an overall porosity of 0.20. However, the coated discs were permeable at room temperature to both helium and hydrogen, therefore we ordered new discs from Refractron.

Discs were ordered from Refractron with a diameter of 1 inch, thickness of 1mm, and pore size of 10 nm. The membrane test assembly was purchased from Pall Corporation and includes a back pressure support screen to prevent the ceramic disc from cracking at high pressure and a Kalrez O-ring to prevent leaks at high temperature. The assembly was tested by placing a stainless steel foil disc over the ceramic disc to ensure that it could hold pressure without leaking. At 100 psig the flow on the permeate side was zero, indicating that at 100 psig, the assembly could be properly sealed.

Subtask 2.3 – Testing Hybrid Metal/Polymer Membrane for Hydrogen Permeation Performance

Synthesized membranes: two sheets of #16: thermally treated before sputtering (16-TT-1) and thermally untreated (16-TU-1) and two of # 20 samples: thermally treated before sputtering (20-TT-1) and thermally untreated (20-TU-1) were tested for gas permeation. Permeation flux data for helium and hydrogen are shown in Table 4. All four membranes show similar high permeation flux values and no hydrogen selectivity is observed. Based on these test results, it can be concluded that metal layers deposited on the support are not dense, and there are still open pores, which allow gases to permeate through the membrane.

Table 4 Permeation Properties of Synthesized Membranes

Membrane	Thickness of Pd-V/Ni-Pd layers, μm	Thermal treatment	Ion assist during sputtering process	H_2 /He flux, mol/cm^2-min
16-TT-1	1-3-1	+	-	419/432
16-TU-1	1-3-1	-	-	417/432
20-TT-1	1-3-1	+	-	406/408
20-TU-1	1-3-1	-	-	419/419
16-with i/s	0.5-1-0.5	-	+	0/0
16-without i/s	0.5-2-0.5	-	-	0/0
20- with i/s	0.5-1-0.5	-	+	0/0
20-without i/s	0.5-2-0.5	-	-	0/0
16/1	0.1-3-0.1	-	+	0/0
16/2	0.05-3-0.05	-	+	0/0
20/1	0.1-2-0.1	-	+	0/0
20/2	0.0.5-2-0.05	-	+	0/0

Due to no difference in permeation fluxes of membranes deposited on thermally treated and thermally untreated supports and their similar stability, no thermal treatment was done before sputtering for subsequent samples.

Based on permeation results, parameters for the sputtering process were changed to deposit more dense metal coating on substrates. Four more membranes were synthesized using membranes: two sheets of #16 (with and without ion source) and two of # 20 samples (with and without ion source). Thicknesses of layers, in case with ion source assistance, are 0.5 µm Pd, 1 µm Ni-V, and 0.5 µm Pd. Two other membranes have the same thickness for Pd layer, but Ni-V layer's thickness equals 2 µm. Permeation flux data for helium and hydrogen are shown in Table 4. All four membranes show no helium and hydrogen fluxes at 250 ºC and pressure difference 200 psi. Based on literature data palladium has lower permeability at these conditions than V-Ni layer, so the next step was to reduce Pd layer thickness from 0.5 microns to 0.1 and 0.05 microns keeping thickness of V-Ni layer the same. The synthesized membranes (16/1, 16/2, 20/1, 20/2) show no hydrogen or helium permeability. Higher feed pressure and higher temperature did not affect the performance.

To understand why membranes are not permeable, energy-dispersive X-ray spectroscopy was used to determine the chemical composition of the metal layer, specifically to identify metal oxides. An SEM image of the membrane is shown in Figure 9. EDS measurements were taken at points shown on the image labeled "Spectrum x". The EDS measurements give the chemical composition at a specific point, with a radius of 1 µm. The concentrations at the points measured are shown in Table 5. The results showed the presence of oxygen in some places where vanadium was detected, indicating that the vanadium is in the oxide form. Where both vanadium and oxygen were detected, the O/V ratio was 1.2. There was no oxygen detected in the palladium layer. Vanadium oxide is impermeable for any gases. That can explain the zero permeation fluxes for synthesized membranes. To reduce the oxide layer, membranes should be subjected to high temperatures (700-800 ºC) in a reducing environment, in which porous polymer supports would not be able to survive.

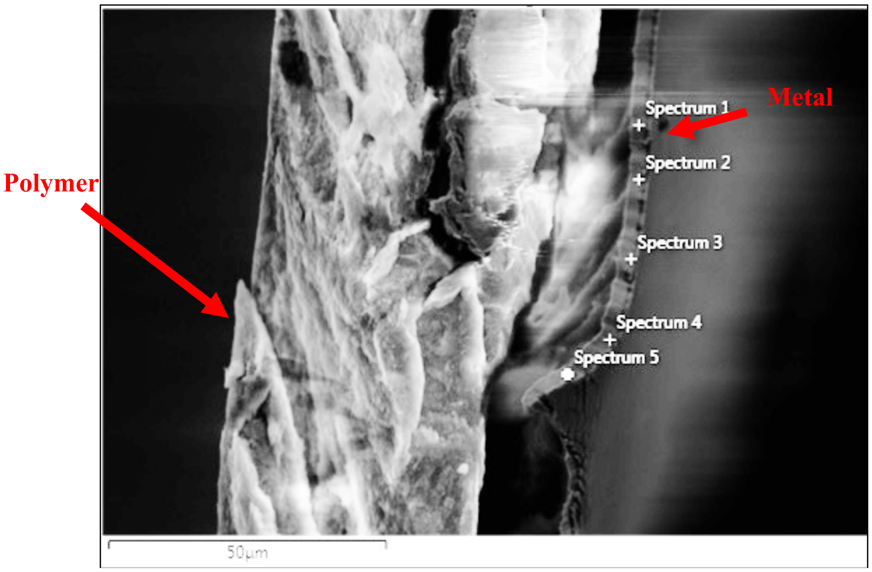


Figure 9 SEM image of synthesized membrane

Table 5 Composition of Metal Layer at Various Points

	Pd	V	O	Ni	Al
Spectrum 1	99	1			
Spectrum 2	12	78		9	
Spectrum 3		37	45	9	8
Spectrum 4		36	44	11	9
Spectrum 5		90		9	

Locations given on Figure 9. *Values given in weight percent*

The thermal stability of the polymer substrate layer (without metal) was tested. The substrate was placed in the testing apparatus under a flow of helium and the permeability of the membrane was tested at different temperatures. The permeability as a function of temperature and time are shown in Figure 10. As the temperature increased, the permeability decreased and permeation dropped to 90 mL/min at 350 °C. As the substrate was held at that temperature the permeation decreased to 44 mL/min after 33 minutes at 350 °C (pressure on the retentate side was constant). This is likely due to expansion of the polymer as it is heated, which blocks the micropores in the substrate. Due to the thermal instability of porous network in substrate, these porous supports cannot be used for hydrogen separation at higher temperatures and extended periods of operations.

Upon receiving the ceramic discs which were ordered to have a diameter of 1 inch and a pore size of 10 nm, we tested them to make sure that the properties met specifications. This was done by placing the discs in the assembly and introducing helium at room temperature. The back pressure regulator was used to apply pressure to the system. The discs were placed in the assembly; they were not able to hold pressure, indicating that the pore size was much larger than expected. We contacted the vendor and they informed us that the discs were made with a pore size of 150 nm, rather than the specified 10 nm pore size. These pores were too large to coat with the Pd and Ni-V layer because it would require a very thick metal layer, which would significantly reduce transport through the membrane and as result, hydrogen permeation values will be lower than DOE target value. Due to time limit, reordering of new porous supports with smaller pore size and synthesis of membranes by metal sputtering was not possible.

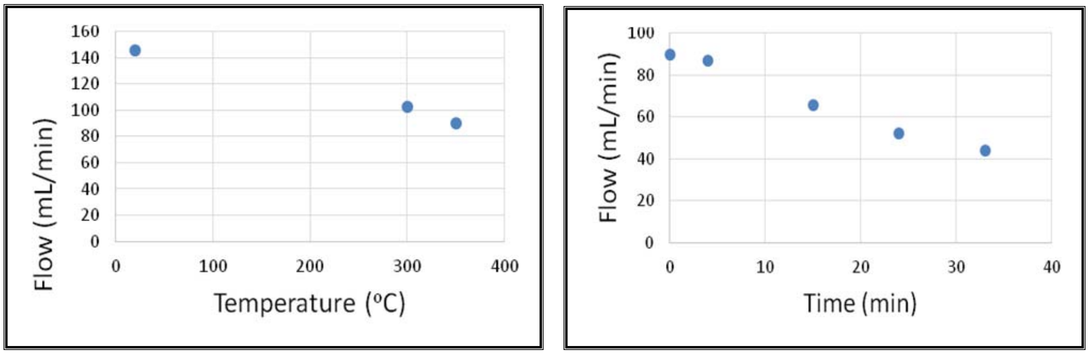


Figure 10 Impact of Temperature and Time on Permeability of Polymer Substrate (without metal layer)

Task 3.0 –Extended Design Data of an Integrated Multi-Component Syngas Impurity Removal Process

Subtask 3.1 – Testing the UCSRP-HP Process for Low-level Sulfur Removal

In this subtask H_2S removal testing was done to simulate the 1st of the 2 stage reactor system for sulfur removal using SR^2. Those results indicated that with inlet H_2S concentration of ~6000 ppmv, the outlet gas stream from the 1st stage reactor could be reduced to ~40-500 ppmv. Using Design of Experiments (DoE) the test plan within the parameters specified in the project objectives was derived and executed to give the results shown in Table 6.

Table 6 Test Plan for Low Inlet H_2S Removal

Pressure, psig	Gas flow	Liquid flow	Temp, °F	Inlet H_2S, ppmv	Inlet SO_2, ppmv	Excess H_2S, %
100	-	-	250	80	38	5
100	-	+	250	80	38	5
100	c	-	250	80	38	5
100	c	+	250	80	38	5
400	+	-	250	80	38	5
400	+	+	250	80	38	5
400	++	-	250	80	38	5
400	++	+	250	80	38	5

The results in Table 7show that more than 95%+ conversion of H_2S even with such low inlet H_2S concentrations resulting in less than 4 ppmv H_2S in the 2nd Stage outlet gas stream.

Table 7 Low-Level Sulfur SR^2 Results

Exp #	Pressure psig	inlet $[H_2S]$ ppmv	Inlet $[SO_2]$ ppmv	Outlet $[H_2S]$ ppmv	Outlet $[SO_2]$ ppmv	H_2S conv. %
1	399	73.0	33.0	2.3	2.5	96.9
2	401	73.0	33.0	1.3	9.5	98.3
3	397	80.6	37.8	3.2	5.0	96.0
4	398	80.6	37.8	1.8	3.3	97.7
5	100	83.7	39.5	1.8	2.1	97.9
6	102	83.7	39.5	3.3	5.6	96.0
7	101	81.3	38.7	2.8	3.4	96.6
8	100	80.0	38.0	3.7	3.0	95.4
9	101	80.0	38.0	2.4	2.5	97.0

Subtask 3.2 – Testing the UCSRP-HP Process for Trace Component Removal

The purpose of the subtask was to identify which solvent among DEG, DGM and water can be used for NH_3 and HCl removal using the same down-flow, co-current reactor with SMV packing used for sulfur tests described in Subtask 3.1. Table 8 shows that at high superficial velocity (2 ft/s) HCl removal was less than 80% when water is used as a solvent. When a superficial gas velocity was decreased to 1 ft/s but with the same water flowrate, target value for HCl removal was achieved. Hence, remaining experiments were done at a superficial gas velocity of1 ft/s. Experiment # 3 was done to show reproducibility of experimental work.

Table 8 Testing SR^2 for Trace Component Removal (HCl)

Exp #	Pressure psig	gas flow scfh	Superficial gas velocity ft/s	Solvent	L/G mass ratio	inlet [HCl] ppmv	Outlet [HCl] ppmv	HCl removed %
1	399	790	2	water	3.3	35.3	10.8	69.4
2	401	355	1	water	7.3	36.1	0.04	99.9
3	397	356	1	water	7.3	38.8	0.08	99.8
4	398	355	1	water	2.4	38.8	0.9	97.7
5	401	359	1	DEG	7.9	43.3	0.04	99.9
6	405	360	1	DEG	2.6	41.8	0.12	99.7
7	400	358	1	DGM	2.4	42.1	0.11	99.6
8	403	355	1	DGM	7.3	43.9	0.02	99.9

Solvents as DEG and DGM show high degrees of HCl removal at the same conditions. Table 8 demonstrates that all three solvents can be used efficiently for HCl removal (>97%) at superficial gas velocity of 1 ft/s.

Table 9 Testing SR^2 for Trace Component Removal (NH_3)

Exp #	Pressure psig	gas flow scfh	Superficial gas velocity ft/s	Solvent	L/G mass ratio	inlet [NH_3] ppmv	Outlet [NH_3] ppmv	NH_3 removed %
9	400	360	1	DGM	7.7	38.5	20.4	47.0
10	405	355	1	DGM	7.8	25.3	11.1	56
11	407	360	1	DGM	2.6	25.7	18.2	29
12	401	351	1	DEG	7.9	26.5	6.9	74.0
13	400	351	1	DEG	2.6	27.5	10.5	61.8
14	403	351	1	Water	7.9	26.0	3.2	87.7
15	399	352	1	Water	2.6	27.8	2.9	89.6

For NH_3 removal testing GTI used the same conditions as in HCl removal experiments: superficial gas velocity of 1 ft/s, the same liquid flow rates and the same inlet NH_3 concentration (see Table 9). Due to low degree of NH_3 removal shown in Experiment #9, inlet NH_3 concentration was reduced (Experiments #10-13) which leads to higher value of the removal efficiency, but lower than target value. Experiments #15 and 16 show water performance as a solvent and demonstrate that water is best solvent for NH_3 removal. Based on the results in Table 8 and Table 9, it is clear that water is a good performing solvent when either HCl or NH_3 are treated. However, syngas derived from coal (e.g. IL #6), contains both components as well as other contaminants at the same time. It is reasonable to assume that both HCl and NH_3 will be removed more efficiently with all three solvents due to reaction between components shown below: $NH_3(g) + HCl(g) = NH_4Cl(aq)$.

Task 4.0 – Conceptual Design and Techno-Economic Evaluation of Low Cost High-H_2 Syngas Production System

Using data from the R&D efforts, we conducted conceptual designs and techno-economic analysis (TEA) to estimate plant efficiency, product costs, and environmental performance for three base-case process configurations involving the Advanced Compact Coal Gasifier and natural gas partial oxidation reactor and the SR^2 technologies for: IGCC plant, chemical-grade hydrogen, and production of liquids fuels, primarily diesel using a Fischer-Tropsch technology, all with carbon capture. Syngases are generated via gasification of Illinois #6 coal and partial oxidation of natural gas with the coal contributing >50% of the total caloric value in the plant. All designs achieved at least 90% carbon capture. Due to the unsuccessful R&D results on the hybrid membrane, conventional technologies were used for carbon capture (single-stage Selexol) and hydrogen purification (PSA) as appropriate in these studies.

All three cases used GEE coal gasifiers in quench mode as their base technology. While the design and material and energy balances around the gasification island are very similar with the same coal feed rate and CO_2 captured rate, there were significant changes in the costs and economic calculations between the IGCC cases, based on [3] and the hydrogen cases, based on [5]. These differences are shown in Table 10. The general design criteria for all cases are given in Appendix A.

Table 10 Key Differences Between Hydrogen and IGCC Study Bases

Design Case	Hydrogen Production	IGCC Power Plant
Reference Basis	[5]	[3]
Coal Feed Rate, TPD	5,301	5,301
Captured CO_2, TPD	10,958	10,951
CAPEX, $ MM		
Coal Handling and GE Gasifier	$511	$395
ASU and Oxidant Compression	251	271
CO_2 Compression & Drying	42	81
Ash/Sorbent Handling	78	54
Economic Factors		
Pricing Basis	First year cost	Levelized cost
Capital Charge Factor, % of TOC	24.9	12.4
Plant Operating Factor, %	90	80

Common Description for GTI Gasification Island

A proprietary AR coal extrusion feed system is utilized for feeding dried coal to the gasifier. Gasifier train in the AR process requires carbon dioxide as coal transport gas as well as steam injection. The AR process claims an adiabatic flame temperature of ~2,600 °F, 1,000 psig operating pressure, and near 100% carbon conversion. The slag, consisting of essentially 100% ash, is removed from the gasification reaction products as hot syngas and molten solids from the reactor flow downward into a radiant cooler where the syngas is cooled and the ash solidifies.

Raw syngas continues downward into a quench system and then into a syngas scrubber for removal of entrained solids. The syngas temperature exiting the quench is approximately 410 °F. Capital and operating costs were derived from [2] and from private communications from AR.

Natural gas, 95% pure O_2 from the ASU, and steam are fed to a non-catalytic, partial oxidation reactor. GTI used Aspen HYSYS software to model the performance of the POX based on literature data from Shell's POX technology that has been commercialized for two plants, as well as data obtained from an ARPA-E sponsored pilot-plant testing program. [7] The pressure and temperature at the POX reactor outlet were 800 psia and 2,400 °F, respectively. The syngas is cooled in a waste heat boiler (WHB) to raise high pressure steam that is directed to the steam turbine. Then, the natural gas-derived syngas is mixed with the coal-derived syngas in the scrubber. Capital and operating costs were derived from [7] and from private communications from AR. A few potential advantages of the proposed GTI Advanced POX concept over a conventional Catalytic-Autothermal Reforming (ATR) unit are:

- For a given plant capacity, the POX combustor volume would be significantly smaller. The POX reactors would be operated at gas residence times of less than 100 milliseconds.
- The concept is amenable to standardized shop-fabrication of highly compact modules of the POX combustor for shipment to plant sites. This could significantly reduce the overall CAPEX requirements for the syngas production step relative to conventional ATR/POX and SMR processes.
- Unlike a catalytic-ATR, there are no requirements for a catalytic pre-reformer, used typically to treat NG containing relatively high levels of C_2- C_4 hydrocarbons, upstream of the ATR, nor for the use of a reforming catalyst in the ATR.
- The POX reactor would most likely be operated at significantly lower steam/carbon (S/C) molar ratio than that typically needed (~0.6) for a catalytic ATR. Moreover, if required, the Advanced POX can be operated at relatively higher outlet temperatures of ~2,400 °F vs. ~2,000 °F maximum for a Catalytic-ATR to increase methane conversion to syngas at a given operating pressure. This would minimize the need for recycling a part of the unconverted NG back to the POX unit, thereby reducing its volume as well as O_2 need for the POX step.

Common Description for GTI SR^2 Island

The syngas stream at 745 psia and 165 °F is processed in a high-pressure co-current down-flow SR^2 Water Scrubbing unit to separate a large fraction of water present in the gas along with NH_3 and halogens and to remove a high fraction of heavy metals. Following this step, the gas is preheated to about 250 °F prior to its processing in the sulfur reactors. The key objective for the removal of a large fraction of the water prior to the sulfur reactors is to minimize the cost of separation of water from DGM solvent used in the reactor. In previous designs, NH_3, halogens, and heavy metals were removed in a DEG Contactor unit.

Heavy metals are collected by three means, namely the primary means: special water filters used following a special high-pressure Water Scrubbing unit in the Gas Cooling/BFW Heating Block located downstream of the Water Gas Shift (WGS) unit, and two conservative backup means: a DURCO liquid sulfur filter, and hydrocyclone/precipitation filters to process a slip-stream of the recycle solvent from the sulfur reactors.

In the sulfur removal and recovery section, the SR^2 absorber/reactor is operated as a co-current down-flow absorber. Based on feed syngas quality, such reactors can be operated with about 10-15% excess (relative to the stoichiometric requirement) of SO_2 or H_2S in the total effluent product gas plus liquid streams to drive the sulfur formation Claus reaction to completion. The elemental sulfur formed is liquid and quickly separates from the less dense solvent. This allows the Claus reaction to continue. Based on experimental data at GTI, it seems that a small quantity of COS, ~10-15% of the H_2S or SO_2 level in the gaseous product at the reactor outlet, might form in such reactors. However, the extent of COS formation appears to be controllable by the presence of water vapor and SO_2 in the product gas with H_2S and CO_2. For the specific feed gas quality and coal properties used in the GTI Base Case studies, the H_2S and COS levels in the product gas from the reactor is <8 ppmv; this will result in a SO_2 emission of about 34 lb/hr from the power plant. As this SO_2 emission level is significantly less than that specified (56 lb/hr) in the DOE IGCC Case, COS hydrolysis reactors may not be required. However to minimize risk, COS hydrolysis reactors and sulfur guard beds were included in the design and costs to bring the sulfur concentrations of the treated syngas/hydrogen stream to <1 ppb.

The product syngas from the SR^2 reactor is cooled to about 90 °F for heat integration, minimization of the loss of DGM solvent with the product syngas and to match the DOE Case conditions. The cooled gas is sent to a high-pressure separator to recover DGM solvent which is processed in a distillation unit to remove the water formed in the reactor due to the reaction of H_2S and SO_2. The syngas is then treated in a single-stage Selexol Unit for CO_2 capture. Liquid SO_2 for reaction with H_2S in the SR^2 reactors is generated by the use of a portion of the sulfur product in a commercial O_2/sulfur submerged combustion furnace as offered by Calabrian Corporation.

Subtask 4.1 – Integrated Gasification Combined Cycle (IGCC) Case

GTI investigated the technical and economic feasibility of a system approach for producing electrical power from coal and natural gas. To satisfy DOE goals, the applied technologies need to be ready for first-of-a-kind commercially relevant demonstration by 2030. This subtask addresses the production of power from coal and natural gas for a nominal 500 MW_e IGCC power plant. All costs are reported in 2013 US dollars.

The DOE IGCC Base Case for the current study is based on DOE/NETL Case B5B-Q published [3] data for the technical and economic feasibility of power generated from bituminous coal. For the DOE IGCC Base Case:

1. Syngas Production:
    a. A GEE Slurry Feed, Oxygen-blown, Quench Coal Gasifier with 100% of the total energy input provided from Illinois No. 6 bituminous coal (Herrin Seam, Old Ben Mine). The syngas is quenched and scrubbed.
2. Sour WGS reactor where >99.99% carbon monoxide reacts with steam to produce carbon dioxide and hydrogen, and >99% of carbonyl sulfide is converted to hydrogen sulfide.
3. A WHB for cooling the intermediate temperature syngas to 275 °F for the production of HP steam used primarily for electric power generation.

4. Conventional mercury removal adsorption, two-stage Selexol process for the removal of H_2S and CO_2, and Claus, hydrogenation, and recycle for sulfur recovery. The captured CO_2 is compressed to 2,215 psia for sequestration.
5. Heating and sending the sweet, clean syngas to a syngas expander and a combined cycle power island with gas and steam turbines to raise electrical power for the plant and export.

The GTI Advanced Case, referred to as the GTI IGCC Case, uses coal and natural gas as the plant energy inputs. For the GTI IGCC Case:

1. Syngas Production:
    a. Fifty one percent of the total energy input is supplied by coal via gasification based on the GTI's Compact Gasification technology. The syngas is quenched and scrubbed.
    b. The remaining 49% of the total energy input is supplied by pipeline-quality natural gas via a separate POX reactor based on the Compact Gasification technology. The high temperature syngas from the POX reactor is cooled in a separate WHB for the production of HP steam used primarily for electric power generation.
2. Sour WGS reactor where >99.99% carbon monoxide reacts with steam to produce carbon dioxide and hydrogen, and >99% of carbonyl sulfide is converted to hydrogen sulfide.
3. WHB for cooling the intermediate temperature syngas to 275 °F for the production of HP steam used primarily for electric power generation.
4. GTI's SR^2 technology then removes and recovers H_2S from the syngas. Multiple contaminants, including mercury, arsenic, and other heavy metals, ammonia and chlorides, are also removed. The SR^2 process is further integrated with COS hydrolysis as well a ZnO-based H_2S guard-bed for the removal of trace-amounts of H_2S prior to a single-stage Selexol-based CO_2 capture step. The captured CO_2 is compressed to 2,215 psia for sequestration.
5. Heating and sending the sweet, clean syngas to a syngas expander and a combined cycle power island with gas and steam turbines to raise electrical power for the plant and export..

DOE/NETL has published data for the technical and economic feasibility of PWR gasification technology for IGCC [2]. This report compared the AR compact gasifier with the GEE gasifier in IGCC without carbon capture. Detailed studies of the GEE gasifier for IGCC with carbon capture were published in [3]. Design and costs for the POX system were derived from [7] and from private communications from AR. The design and economics of SR^2 process was published [4]. These reports served the basis for current study.

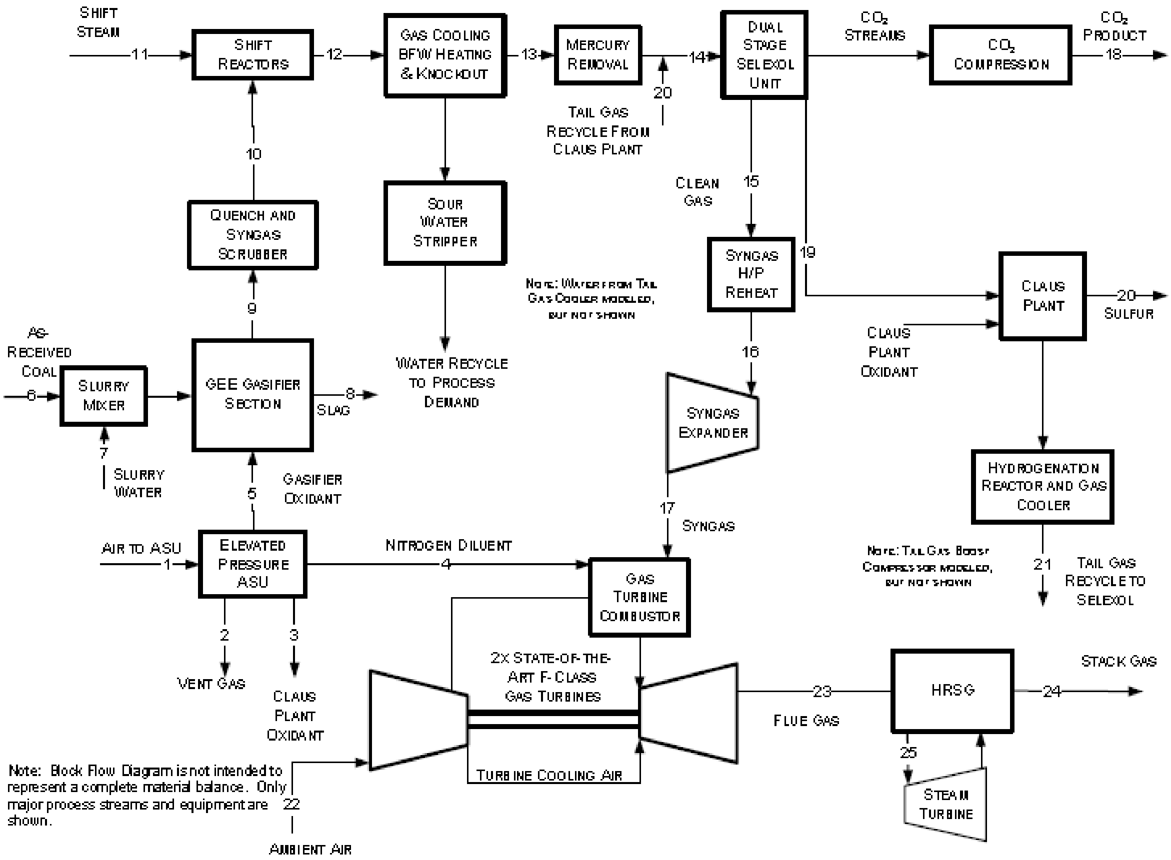


Figure 11 DOE IGCC Base Power Production Plant Block Flow Diagram

A schematic of the overall flowsheet of the DOE IGCC Base Case is shown in Figure 11. Consuming 5,301 TPD of Illinois No. 6 coal (as received), the GEE coal gasification IGCC plant produces 492 MW_e. The plant requires a total auxiliary load of 191 MW_e. The total plant capital cost is estimated to be \$1,630 MM. At an 80% capacity factor, the Levelized Cost of Electricity (COE) with TS&M is \$134/MW_e.

In the GTI IGCC Case, we have evaluated the economic potential of producing a high hydrogen syngas from gasification of coal and partial oxidation of natural gas. For the 514 MW_e power plant, AR gasifiers are used to gasify 2,634 TPD of Illinois No. 6 coal (as received) to produce syngas that is blended with syngas produced from 1,393 TPD of natural gas fed to a separate, non-catalytic partial oxidation (POX) reactor. The overall energy input to this plant is 51% from coal and 49% from natural gas. The plant requires a total auxiliary load of 168 MW_e. The total plant capital cost is estimated to be \$1,291 MM. At an 80% capacity factor, the Levelized COE with TS&M is \$127/MW_e, about 5% less than the base case.

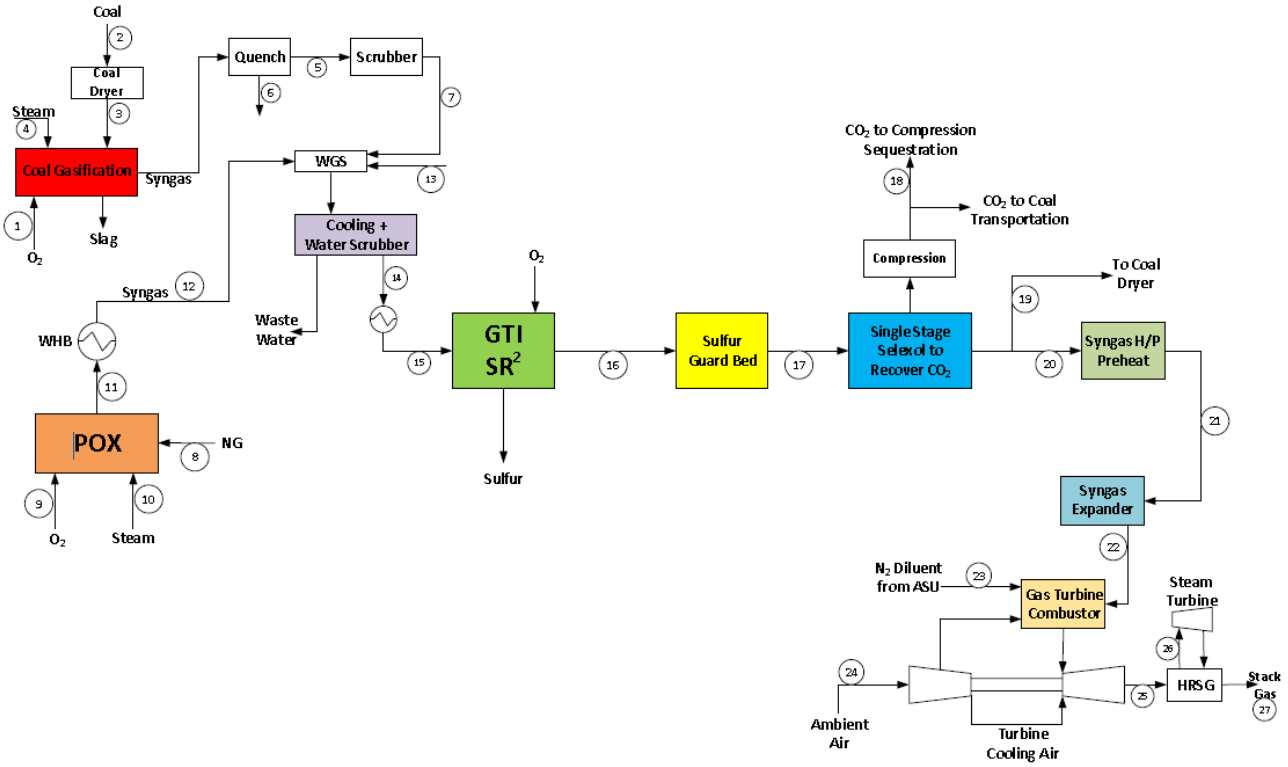


Figure 12 GTI IGCC Case Power Production Plant Block Flow Diagram

A schematic of the proposed hybrid feed concept is shown in Figure 12. The syngas from the Advanced Compact coal gasification section is quenched and scrubbed as described in Reference [2]. Pipeline-quality natural gas is processed in a non-catalytic Advanced POX reactor to produce a syngas at 2400 °C. This POX syngas is cooled in a separate WHB to raise high pressure steam. The coal-derived syngas is blended with the intermediately cooled syngas from the POX WHB unit for processing in a shift reactor (WGS). The WGS syngas-effluent is further processed in the SR^2 unit for the removal of H_2S and other key contaminants such as chlorides, arsenics and mercury. The syngas effluent with a H_2S plus COS content of <8 ppmv is further treated in a Sulfur Guard-bed unit/COS hydrolysis step as needed to eliminate trace-levels of sulfur compounds. The treated syngas is then processed in a single-stage Selexol unit for the removal of most of the CO_2 prior to the power island. The CO_2-rich gas (CO_2 >95% by volume) is compressed to ~2,200 psia and dried for sequestration. The syngas, now predominantly hydrogen, is combusted for power in the same power island design as in the DOE IGCC flowsheet. The material balances for the key streams are shown in Table 11. The material balances for the Advanced Compact coal gasifier were provided by AR; those for the POX reactor were estimated by GTI using Aspen HYSYS software and experimental work performed under an ARPA-E study. Sulfur removal and recovery, as well as removal of trace components such as arsenics, chlorides, and mercury, is performed using GTI's SR^2 process. The DOE IGCC Case captured 10,958 TPD CO_2 while the GTI IGCC Case captured 8,957 TPD CO_2, about 18% less.

Table 11 GTI IGCC Case Production Plant Streams

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
V-L Mole Fraction												
Ar	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.931	0.000	0.000	0.001	0.001
CO	0.000	0.000	0.000	0.000	0.280	0.000	0.370	0.000	0.000	0.000	0.287	0.286
CO_2	0.000	0.000	0.000	0.000	0.055	0.000	0.072	0.010	0.000	0.000	0.026	0.029
COS	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000
H_2	0.000	0.000	0.000	0.000	0.113	0.000	0.148	0.000	0.000	0.000	0.543	0.534
H_2O	0.000	0.000	0.000	1.000	0.536	0.000	0.391	0.000	0.000	1.000	0.134	0.150
H_2S	0.000	0.000	0.000	0.000	0.004	0.000	0.004	0.000	0.000	0.000	0.000	0.000
N_2	0.050	0.000	0.000	0.000	0.010	0.000	0.013	0.016	0.050	0.000	0.010	0.001
NH_3	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000
O_2	0.950	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.950	0.000	0.000	0.000
SO_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Others	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.043	0.000	0.000	0.000	0.000
Total	1.000	0.000	0.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000
Temperature , °F	800	59	195	800	745	500	410	1200	572	1200	2400	410
Pressure, psia	1200	1200	1200	1200	805	990	800	800	800	800	800	800
V-L Flowrate, lb/hr	223,564	0	0	355,396	791,060	0	625,925	127,919	163,004	33,534	317,282	317,282
Solid Flowrate, lb/hr	0	241,591	226,611	0	0	23,435	0	0	0	0	0	0

	13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
V-L Mole Fraction												
Ar	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0023	0.0092
CH_4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO_2	0.000	0.361	0.361	0.356	0.356	1.000	0.036	0.036	0.360	0.000	0.000	0.0003
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H_2	0.000	0.623	0.623	0.632	0.633	0.000	0.947	0.947	0.947	0.999	0.000	0.000
H_2O	1.000	0.002	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.0003	0.000
H_2S	0.000	0.003	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N_2	0.000	0.011	0.011	0.011	0.011	0.000	0.017	0.017	0.017	0.000	0.9920	0.7732
NH_3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0054	0.2074
SO_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Others	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Temperature , °F	550	90	275	275	95	124	95	95	465	370	199	59
Pressure, psia	800	755	745	715	700	2,215	700	700	695	460	384	14.7
V-L Flowrate, lb/hr	55,898	995,627	995,627	989,000	987,923	822,802	418	151,363	151,363	151,363	1,159,055	6,556,015
Solid Flowrate, lb/hr	0	0	0	0	0	0	0	0	0	0	0	0

Table 12 Key Comparative Data for IGCC

Design Case	**DOE IGCC Base Case**	**GTI IGCC Case**	**Units**
Coal Feed Rate (as received)	5,301	2,634	TPD
Natural Gas Feed Rate	--	1,393	TPD
Energy from Feed Coal	100	51	%
O_2 Needed	4,343	4,280	TPD
Net Electricity Production	**492.5**	**514.4**	**MW_e**
CO_2 for Sequestration	10,951	8,957	TPD

1. *90% Plant Operating Factor; coal @ $1.70/MMBtu; natural gas @ $4/MMBtu*
2. *The Capital Charge is estimated as 12.4% of TOC*

Comparative plant performance data and the power production/usage data for the two cases are compared in Table 12 and Table 13 respectively. The estimates on capital cost items for determining the total overnight capital cost (TOC) are compared in Table 14 - Table 16. Table 17 provides the key details on the annual O&M costs and the estimates on the cost of electricity with and without CO_2 TS&M.

Thus, the GTI IGCC case with coal plus natural gas case results in 5% lower electricity costs than in the DOE IGCC Base case. Reduction in the capital costs for solids processing, gas clean-up, and gasification using POX of a gas stream instead of exclusively coal gasification more than offsets the higher feed cost ($4/MMBtu for natural gas versus $1.70/MMBtu for coal). The advantage for the GTI IGCC case will grow with higher coal prices and/or lower gas prices.

Table 13 Plant Performance Summary for IGCC

	DOE IGCC Base Case	**GTI IGCC Case**	**Units**
Plant Output -100 Percent Load			
Combustion Turbine Power	464,000	433,700[1]	kW_e
Sweet Gas Expander Power	7,000	5,315	kW_e
Steam Turbine Power	214,000	200,020[1]	kW_e
Steam Turbine from WHB in POX unit		43,500	kW_e
Total	**684,000**	**682,535**	**kW_e**
Auxiliary Load Summary			
Coal Handling/Milling	2,740	1,360	kW_e
Sour Water Recycle Slurry Pump	200	100	kW_e
Slag Handling	1,160	575	kW_e
ASU Auxiliaries	1,000	1,000	kW_e
ASU Main Air Compressor	67,350	67,060	kW_e
Oxygen Compressor	10,640	10,595	kW_e
Nitrogen Compressor	35,630	33,305	kW_e
Feed Water and Quench Water and Scrubber Pumps	4,370	3,060[2]	kW_e
CO_2 Compressor	31,130	25,470	kW_e
Acid Gas Removal	19,210	10,390	kW_e
Combustion Turbine Auxiliaries	1,000	935	kW_e
Steam Turbine Auxiliaries	100	115	kW_e
Various Pumps (Condensate, Circulating Water and Ground Water)	5,620	3,935[2]	kW_e
Cooling Tower Fans	2,500	2,500	kW_e
Claus Plant/TGTU Auxiliaries	250	--	kW_e
Claus Plant TGTU Recycle Compressor	1,800	--	kW_e
WGS Makeup Pump	1,150	950	kW_e
GTI SR^2 System	--	1,100	kW_e
Miscellaneous Balance-of-Plant	3,000	3,000	kW_e
Transformer Losses	2,710	2,705	kW_e
Total	**191,560**	**168,155**	**kW_e**
Plant Performance			
Net Plant Power	**492,440**	**514,380**	**kW_e**
As-received Coal Feed Flowrate	5,301.4	2,634.0	TPD
Natural Gas Flowrate	--	1,392.6	TPD
Thermal Input (HHV basis)	1,664.955	1,673.144	$MW_{thermal}$

1. *Prorated from LHV in Stream #20*
2. *Assume 70% of the DOE Case (GE design uses a slurry feed)*

Table 14 Capital Cost Summary for IGCC

Design Case		DOE IGCC Base Case	GTI IGCC Case
Acct. No.	**Item/Description, $MM**		
1	Coal Receiving/Stackout/Conveyors, other handling/Key Foundations	43.0	--
2	Coal Crushing/Drying, Storage, Slurry-Prep/Feed and specific Foundations	69.0	--
3	Feedwater System, Service water/Boiler Plant units/Waste Treatment Equip. and Misc. Power Plant Equip.	61.0	
4.1/ 4.4/ 4.5 and 4.8/4.9	Gasification Systems	222.3	293.0 (includes Accounts 1, 2 & 3)
4.3	ASU/Oxidant Compression	271.0	271.0
	Subtotal 4	**493.3**	**564.0**
5A	Gas Cleanup & Piping		
5A.1	Selexol unit	244.0	72.2
5A.2	Elemental Sulfur Plant	39.5	--
5A.2	GTI SR^2	--	12.7
5A.3	Mercury Removal	4.6	--
5A.4	Shift Reactors	21.7	15.0
5A.7 and1.9	Fuel Gas Piping/Foundations	3.4	3.4
	Subtotal 5A	**313.2**	**103.3**
5B.2	CO_2 Compression & Drying	81.4	70.7
6.1	Combustion Turbine Generator	152.3	145.3
6.2	Syngas Expander	9.4	7.8
6.9	Combine Turbine Foundations	3.1	3.0
7.1/7.3/ 7.4 and 7.9	Heat Recovery Steam Generator, Duct/Stack, HRSG and Foundations	54.7	52.2
8.1/8.2/8.3 and8.4/8.9	Steam Turbine Generator and Related Systems	78.1	85.5
9	Cooling Water Systems and Foundations	40.4	40.4
10	Ash/Spent Sorbent Handling System	53.8	33.0
11	Accessory Electric Plant	103.0	102.8
12/13/14	Instrumentation/Control and Site Improvements and Buildings	74.0	74.0
15	POX System	--	9.7
	TOTAL PLANT CAPEX	**1,629.7**	**1,291.7**

Table 15 Pre-Production and Inventory Costs

Design Case, all costs in $MM	**DOE IGCC Base Case**	**GTI IGCC Case**
6 Months All Labor	14.85	14.85
1 Month Maintenance Material	3.31	3.31
1 Month Non-fuel Consumables	0.73	0.73
1 Month Waste Disposal	0.52	0.52
25% of 1 Months Fuel Cost at 100% CF[2]	1.76	2.99
2% of TPC	32.6	25.83
Total Pre-Production Costs[1]	**53.77**	**48.23**
60-day Supply of Fuel and Consumables @ 100% CF	15.54	25.34
0.5% TPC (Spare Parts)	8.14	6.46
Total Inventory Capital	**23.68**	**31.80**

1. *Assume 3.6% inflation during 2011 to 2013*
2. *Cost of as-received coal = $1.70/MMBtu (HHV)*

Table 16 Overall Capital Cost Summary for IGCC

Design Case, all costs in $MM	**DOE IGCC Base Case**	**GTI IGCC Case**
Preproduction Costs	53.8	48.3
Inventory Capital	23.7	31.8
Initial Cost for Catalysts/Chemicals	17.3	17.3
Land	1.0	1.0
Other owners cost, 15% of TPC	244.5	193.8
Financing Costs, 2.7% of TPC	44.0	34.9
Subtotal	*384.3*	*327.1*
TOC = Subtotal and Total Plant CAPEX	**2,014.0**	**1,618.8**
Total As-Spent Cost (TOC x 1.201 as [5])	***2,419.0***	***1,944.2***

Table 17 IGCC Power Production Costs

	DOE IGCC Base Case	GTI IGCC Case	Units
O&M Costs			
Total Fixed O&M	64.5	64.5	\$MM/yr
Total Variable O&M	43.6	40.4	\$MM/yr
Annual Fuel Costs	67.65	114.62	\$MM/yr
Total Annual O&M Costs	175.75	219.52	\$MM/yr
Cost of Electricity			
Total Plant CAPEX	1,630	1,292	\$MM
TOC, \$MM	2,014	1,619	\$MM
Net Power	492.44	514.38	MW_e
Capital Charge (12.4% of TOC)	249.75	200.76	\$MM/yr.
Capital related COE	72.4	55.7	\$/MW_e
Fixed-Cost related COE	18.7	17.9	\$/MW_e
Variable-Cost Related COE	12.6	11.2	\$/MW_e
Fuel-Cost related COE	19.6	31.8	\$/MW_e
Total COE, (Excluding TS&M)	123.3	116.6	\$/MW_e
CO_2 TS&M	10.6	10.6	\$/MW_e
Total COE, Including TS&M)	***133.9***	***127.2***	***\$/MW_e***
RELATIVE	***100***	***95***	***--***

1. *The first year Capital Charge is estimated as 12.4% of TOC*
2. *O&M assumed 3.65% increase over the Year 2011 costs given in [3]*

Subtask 4.2 – Chemical-Grade Hydrogen Case

GTI investigated the technical and economic feasibility of a system approach for producing high-purity hydrogen from coal and natural gas. To satisfy DOE goals, the applied technologies need to be ready for first-of-a-kind commercially relevant demonstration by 2030. This subtask addresses the production of high-purity hydrogen (>99.9^+ % purity) from coal and natural gas for a nominal 650 metric tons/day (TPD) of hydrogen plant. All costs are reported in 2013 US dollars.

The DOE Hydrogen Base Case for the current study is based on DOE/NETL Case 2-2 published [5] data for the technical and economic feasibility of hydrogen production. For the DOE Base Case:

1. Syngas Production:
    a. A GEE Slurry Feed, Oxygen-blown, Quench Coal Gasifier with 100% of the total energy input provided from Illinois No. 6 bituminous coal (Herrin Seam, Old Ben Mine). The syngas is quenched and scrubbed.
2. Sour WGS reactor where >99.99% carbon monoxide reacts with steam to produce carbon dioxide and hydrogen, and >99% of carbonyl sulfide is converted to hydrogen sulfide.
3. A WHB for cooling the intermediate temperature syngas to 275 °F for the production of HP steam used primarily for electric power generation.

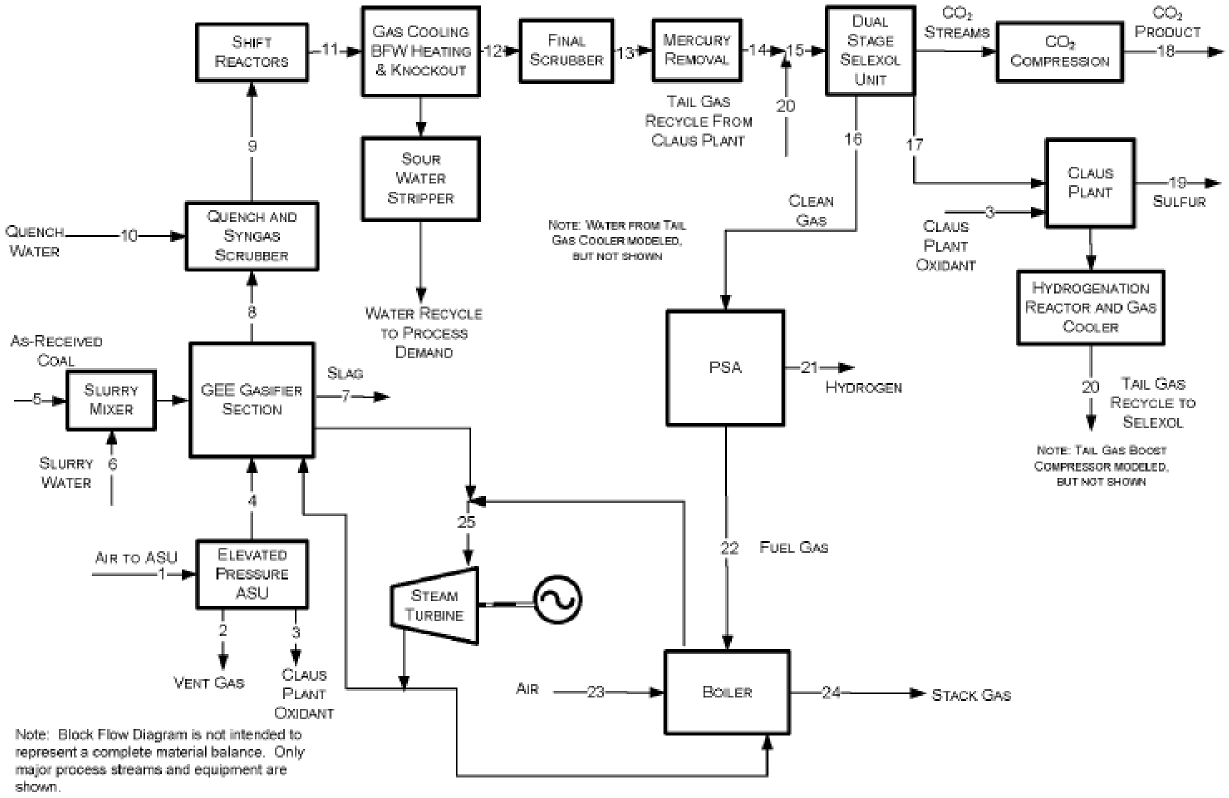
4. Conventional mercury removal adsorption, two-stage Selexol process for the removal of H_2S and CO_2, and Claus, hydrogenation, and recycle for sulfur recovery. The captured CO_2 is compressed to 2,215 psia for sequestration.
5. A conventional PSA for H_2 recovery from treated syngas containing near-zero sulfur and relatively low levels of CO_2 (4 vol.%) and nitrogen (1.7%). The hydrogen is >99.9% pure and the PSA tail gas is used as a fuel gas for the steam boiler.

The GTI Advanced Case, referred to as the GTI Hydrogen Case, uses coal and natural gas as the plant energy inputs. For the GTI Hydrogen Case:

1. Syngas Production:
    a. Fifty one percent of the total energy input is supplied by coal via gasification based on the GTI's Compact Gasification technology. The syngas is quenched and scrubbed.
    b. The remaining 49% of the total energy input is supplied by pipeline-quality natural gas via a separate POX reactor based on the Compact Gasification technology. The high temperature syngas from the POX reactor is cooled in a separate WHB for the production of HP steam used primarily for electric power generation.
2. Sour WGS reactor where >99.99% carbon monoxide reacts with steam to produce carbon dioxide and hydrogen, and >99% of carbonyl sulfide is converted to hydrogen sulfide.
3. WHB for cooling the intermediate temperature syngas to 275 °F for the production of HP steam used primarily for electric power generation.
4. GTI's SR^2 technology then removes and recovers H_2S from the syngas. Multiple contaminants, including mercury, arsenic, and other heavy metals, ammonia and chlorides, are also removed. The SR^2 process is further integrated with COS hydrolysis as well a ZnO-based H_2S guard-bed for the removal of trace-amounts of H_2S prior to a single-stage Selexol-based CO_2 capture step. The captured CO_2 is compressed to 2,215 psia for sequestration.
5. A conventional PSA for H_2 recovery from treated syngas containing near-zero sulfur and relatively low levels of CO_2 (4 vol.%) and nitrogen (1.7%). The hydrogen is >99.9% pure and the PSA tail gas is used as a fuel gas for the steam boiler.

DOE/NETL has published data for the technical and economic feasibility of PWR gasification technology for hydrogen production [2]. This report compared the AR compact gasifier with the GEE gasifier for IGCC without carbon capture. Design and costs for the POX system were derived from [7] and from private communications from AR. Detailed studies of the GEE gasifier for H_2 production with carbon capture were published in [5]. The design and economics of SR^2 process was published in [4]. These reports served the basis for current study.

A schematic of the overall flowsheet of the DOE Base Case H_2 production plant is shown in Table 18. Consuming 5,301 TPD of Illinois No. 6 coal (as received), the GEE coal gasification hydrogen production plant produces 619 TPD of 99.9%+ H_2. The plant requires the import of 35.5 MW_e of power to meet a total auxiliary load of 148 MW_e. The total plant capital cost is estimated to be $1,411 MM. At a 90% capacity factor, the First Year Cost of Hydrogen with TS&M is $3.41/kg. The DOE Hydrogen Case captured 10,951 TPD CO_2 while the GTI Hydrogen Case captured 8,957 TPD CO_2, about 18% less.



Note: Block Flow Diagram is not intended to represent a complete material balance. Only major process streams and equipment are shown.

Figure 14 DOE Hydrogen Base Case Plant Block Flow Diagram

In the GTI Case, we have evaluated the economic potential of producing a high hydrogen syngas from gasification of coal and partial oxidation of natural gas. For the hydrogen production plant (size equivalent to 550 MW_e power plant), AR gasifiers are used to gasify 2,634 TPD of Illinois No. 6 coal (as received) to produce syngas that is blended with syngas produced from 1,393 TPD of natural gas fed to a separate, non-catalytic partial oxidation (POX) reactor for the production of 668 TPD of 99.9%+ hydrogen. The overall energy input to this plant is 51% from coal and 49% from natural gas. The plant requires the import of 14 MW_e of power to meet a total auxiliary load of 131 MW_e. The total plant capital cost is estimated to be $972 MM. At a 90% capacity factor, the First Year Cost of Hydrogen with TS&M is $2.71/kg, about 20% less than the base case.

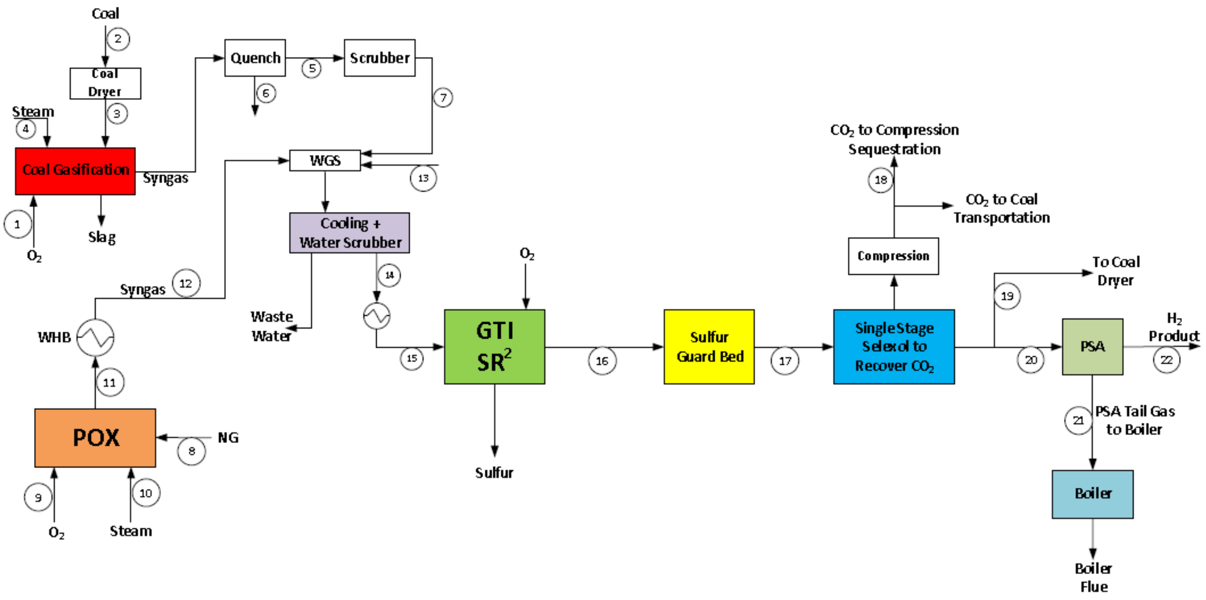


Figure 15 GTI Hydrogen Base Case Plant Block Flow Diagram

A schematic of the proposed hybrid feed concept is shown in Figure 15. The syngas from the Advanced Compact coal gasification section is quenched and scrubbed as described in [2]. Pipeline-quality natural gas is processed in an Advanced POX reactor to produce a syngas at 2400 °C. This POX syngas is cooled in a separate WHB to raise high pressure steam. The coal-derived syngas is blended with the intermediately cooled syngas from the POX WHB unit for processing in a shift reactor (WGS). The WGS syngas-effluent is further processed in the SR^2 unit for the removal of H_2S and other key contaminants such as chlorides, arsenics and mercury. The syngas effluent with a H_2S plus COS level of <8 ppmv is further treated in a Sulfur Guard-bed unit/COS hydrolysis step as needed to eliminate trace-levels of sulfur compounds. The treated syngas is then processed in a single-stage Selexol unit for the removal of most of the CO_2 prior to the PSA unit. The CO_2-rich gas (CO_2 >95% by volume) is compressed to ~2,200 psia for further sequestration. The recovery of hydrogen is about 84% in the PSA unit as used in the DOE case. The tail-gas effluent from the PSA unit is sent to a boiler for the generation of high-pressure steam. The hydrogen product is >99.9% pure. The material balances for the key streams are shown in Table 18. The material balances for the Advanced Compact coal gasifier were provided by AR; those for the POX reactor were estimated by GTI using Aspen HYSYS software and experimental work performed under an ARPA-E study. Sulfur removal and recovery, as well as removal of trace components such as arsenics, chlorides, and mercury, is performed using GTI's SR^2 process.

Table 18 GTI Hydrogen Case Production Plant Streams

	1	2	3	4	5	6	7	8	9	10	11	12
V-L Mole Fraction												
Ar	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.931	0.000	0.000	0.001	0.001
CO	0.000	0.000	0.000	0.000	0.280	0.000	0.370	0.000	0.000	0.000	0.287	0.286
CO_2	0.000	0.000	0.000	0.000	0.055	0.000	0.072	0.010	0.000	0.000	0.026	0.029
COS	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000
H_2	0.000	0.000	0.000	0.000	0.113	0.000	0.148	0.000	0.000	0.000	0.543	0.534
H_2O	0.000	0.000	0.000	1.000	0.536	0.000	0.391	0.000	0.000	1.000	0.134	0.150
H_2S	0.000	0.000	0.000	0.000	0.004	0.000	0.004	0.000	0.000	0.000	0.000	0.000
N_2	0.050	0.000	0.000	0.000	0.010	0.000	0.013	0.016	0.050	0.000	0.010	0.001
NH_3	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000
O_2	0.950	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.950	0.000	0.000	0.000
SO_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Others	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.043	0.000	0.000	0.000	0.000
Total	1.000	0.000	0.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000
Temperature , °F	800	59	195	800	745	500	410	1200	572	1200	2400	410
Pressure, psia	1200	1200	1200	1200	805	990	800	800	800	800	800	800
V-L Flowrate, lb/hr	223,564	0	0	355,396	791,060	0	625,925	127,919	163004	33,534	317,282	317,282
Solid Flowrate, lb/hr	0	241,591	226,611	0	0	23,435	0	0	0	0	0	0

	13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**
V-L Mole Fraction										
Ar	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO_2	0.000	0.361	0.361	0.356	0.356	1.000	0.036	0.036	0.182	0.001
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H_2	0.000	0.623	0.623	0.632	0.633	0.000	0.947	0.947	0.737	0.999
H_2O	1.000	0.002	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.000
H_2S	0.000	0.003	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N_2	0.000	0.011	0.011	0.011	0.011	0.000	0.017	0.017	0.081	0.000
NH_3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SO_2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Others	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Temperature , °F	550	90	275	275	95	124	95	95	20	90
Pressure, psia	800	755	745	715	700	2,215	700	700	77	715
V-L Flowrate, lb/hr	55,898	995,627	995,627	989,000	987,923	822,802	418	151,363	92,405	61,403
Solid Flowrate, lb/hr	0	0	0	0	0	0	0	0	0	0

Table 19 Key Comparative Data for Hydrogen Production

Design Case	DOE Hydrogen Base Case	GTI Hydrogen Case	Units
Coal Feed Rate (as received)	5,301	2,634	TPD
Natural Gas Feed Rate	--	1,393	TPD
Energy from Feed Coal	100	51	%
O_2 Needed	4,324	4,280	TPD
Import of Electricity	35.44	13.98	MW_e
H_2 Produced	**618.9** **25,789**	**668.5** **27,852**	**TPD** **kg/hr**
CO_2 for Sequestration	10,958	8,957	TPD

Comparative plant performance data and the power production/usage data for the two cases are compared in Table 19 and Table 20 respectively. The estimates on capital cost items for determining the total overnight capital cost (TOC) are compared in Table 21 and Table 22. Table 23 provides the key details on the annual O&M costs and the estimates on the first-year production cost of hydrogen with and without CO_2 TS&M.

Table 20 Plant Performance Summary for Hydrogen Production

	DOE Hydrogen Base Case	**GTI Hydrogen Case**	**Units**
Plant Output -100 Percent Load			
Steam Turbine Power from WHB in Coal Gasification Section	112,700	15,000	kW_e
Steam Turbine Power from WHB in the POX Section		43,500	kW_e
Steam Turbine Power from Tail Gas from PSA unit		58,400	kW_e
Total	**112,700**	**116,900**	$\mathbf{kW_e}$
Auxiliary Load Summary			
Coal Handling/Milling and Slag Handling	3,900	1,140	kW_e
Coal Slurry Pumps	200	--	kW_e
ASU Auxiliaries	1,000	990	kW_e
ASU Main Air Compressor	67,050	66,370	kW_e
Oxygen Compressor	10,580	10,470	kW_e
CO_2 Compressor	31,150	26,325	kW_e
Feed Water Pumps	1,690	1,750	kW_e
Various Pumps (Condensate, Quench water, Circulating water and Ground water and Scrubber)	5,290	5,490	kW_e
Cooling Tower Fans	1,590	1,590	kW_e
Acid Gas Removal	19,220	10,390[1]	kW_e
Claus Plant/TGTU Auxiliaries	250	--	kW_e
Steam Turbine Auxiliary	100	105	kW_e
Claus Plant TGTU Recycle Compressor	1,940	--	kW_e
WGS Makeup Pump	--	950	kW_e
Boiler Air Compressor	305	305	kW_e
GTI SR^2 System	--	1,100	kW_e
Miscellaneous Balance-of-Plant	3,000	3,000	kW_e
Transformer Losses	870	900	kW_e
Total	**148,135**	**130,875**	$\mathbf{kW_e}$
Plant Performance			
Net Plant Power	**-35,435**	**-13,975**	kW_e
H_2 (>99.9%+) Production	618.9	668.5	TPD
As-received Coal Feed Flowrate	5,301.4	2,634.0	TPD
Natural Gas Flowrate	--	1,392.6	TPD
Thermal Input (HHV basis)	1,664.955	1,673.144	$MW_{thermal}$

3. Single Stage CO_2 removal based on [4]

Table 21 Capital Cost Summary for Hydrogen Production

Design Case		DOE Hydrogen Base Case	GTI Hydrogen Case
Acct. No.	**Item/Description, $MM**		
1 and2	Coal Handling and Coal Prep/Feed System	103.9	56.3
3	Feedwater & Misc. BOP System	21.6	6.3
4	Gasification Island		
4.1 and 4.2	Gasification Systems	368.0	230.0
4.3	ASU/Oxidant Compression	251.3	250.0
4.4-4.9	Other Gasification Systems	17.4	(included in 4.1/4.2
	Subtotal 4	636.7	480.0
5A	Gas Cleanup & Piping		
5A.1	Selexol Unit	231.5	72.2
5A.2	Elemental Sulfur Plant	36.8	--
5A.2	GTI SR^2	--	12.7
5A.3	Mercury Removal	3.7	--
5A.4	Shift Reactors	20.2	13.9
5A.7 and1.9	Fuel Gas Piping/Foundations	3.1	3.1
	Subtotal 5A	295.3	101.9
5B	CO_2 Compression & Drying	42.0	37.3
6	PSA Unit for H_2 Production	57.8	61.0
7	Off-gas Fired Boiler & Stack	31.5	25.9
8	Steam Turbine Generator	37.1	38.1
9	Cooling Water System	19.1	19.6
10	Ash/Spent Sorbent Handling System	77.7	47.6
11	Accessory Electric Plant	23.0	23.6
12/13/14	Instrumentation/Control and Site Improvements and Buildings	65.2	65.2
15	POX System	--	9.7
	TOTAL PLANT CAPEX	**1,410.9**	**972.5**

Table 22 Overall Capital Cost Summary for Hydrogen Production

Design Case, all costs in $MM	**DOE Hydrogen Base Case**	**GTI Hydrogen Case**
Preproduction Costs	47.9	40.4
Inventory Capital	8.0	5.8
Initial Cost for Catalysts/Chemicals	7.9	7.9
Land	1.0	1.0
Other owners cost, 15% of TPC	211.7	145.9
Financing Costs, 2.7% of TPC	38.1	26.3
Subtotal	314.6	227.3
TOC = Subtotal and Total Plant CAPEX	**1,725.5**	**1,199.8**
Total As-Spent Cost (TOC x 1.201)	**2,072.3**	**1,441.0**

Table 23 Hydrogen Production Costs

	DOE Hydrogen Base Case	**GTI Hydrogen Case**	**Units**
O&M Costs			
Total Fixed O&M[1]	53.0	53.0	$MM/yr
Total Variable O&M[1]	87.0	64.7	$MM/yr
Annual Fuel Costs	76.1	128.945	$MM/yr
Total Annual O&M Costs	216.1	246.645	$MM/yr
Cost of Hydrogen			
Total Annual Costs (excluding capital)	216.1	246.7	$MM/yr
First Year Capital Charge (24.9% of TOC)	429.7	298.8	$MM/yr
Total annual production costs	645.8	545.5	$MM/yr
H_2 Production	618,940	668,453	kg/day
First Year H_2 Cost, without CO_2 TS&M[2]	**3.18**	**2.48**	**$/kg**
First Year H_2 Cost, (with CO_2 TS&M) **RELATIVE**	**3.41** **100**	**2.71** **79.5**	**$/kg** **--**

1. *Assume 12.5% increase over the Year-2007 costs as reported in the DOE Report*
2. *The first year Capital Charge is estimated as 24.9% of TOC*

Subtask 4.3 – Production of Diesel Case

DOE/NETL has published data for technical and economic feasibility of a small-scale coal-to-liquids (CTL) facility (nominal 10,000 BSD of liquids) in southwestern West Virginia [1]. The facility employs gasification and Fischer-Tropsch (FT) technology to produce commercial-grade zero-sulfur diesel and naphtha from a high-sulfur bituminous coal. For the design estimates, coal/water slurry-fed GE gasifiers were used to gasify ~3,628 TPD of dry Pittsburgh No. 8 coal to produce syngas for the production of ~9,609 BSD of diesel and naphtha with ~56 vol. % of the liquid product being diesel. For that study, the H_2/CO molar ratio of the syngas from a scrubber unit was estimated at ~0.80. Following additional clean-up for the removal of various contaminants including H_2S and mercury, the syngas feed to the FT plant contained a H_2/CO ratio of ~0.81. A schematic of the overall flow-sheet of the gasification/FT concept is shown in Figure 17.

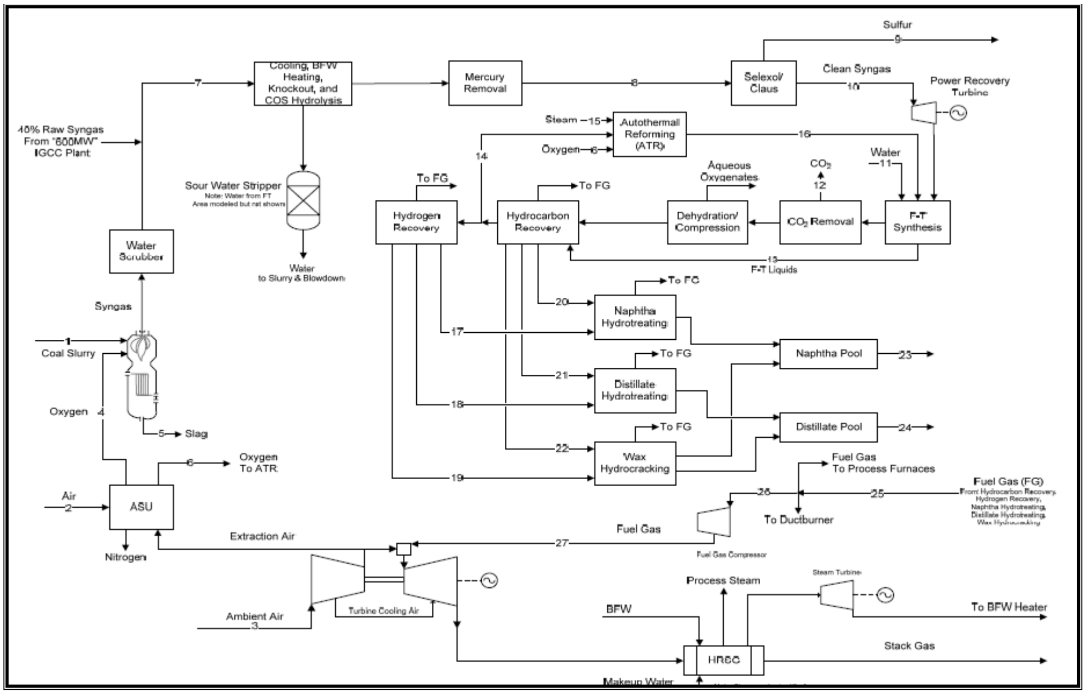


Figure 17 DOE CTL Base Case Flowsheet for the Production of Diesel and Naphtha from Coal

We have evaluated the economic potential of producing a part of the syngas by gasifying Illinois #6 coal using an AR coal gasifier that uses a proprietary coal extrusion feed system for feeding near-dry coal (containing ~ 5 wt% moisture) to the gasifier, and the rest of the syngas from natural gas, mixed with steam and oxygen, in a separate non-catalytic partial oxidation (POX) reactor. Shell's POX technology has been commercialized for two plants. Design and costs for the POX system were derived from [7] and from private communications from AR. The syngas from AR coal gasification has a H_2/CO ratio of about 0.4 and we have used natural gas partial oxidation, with some CO_2 recycle, to generate specific syngas composition so that the fresh mixed syngas feed to the FT reactor has the same composition as in DOE Case [1].

A schematic of the proposed hybrid feed concept is shown in Figure 18. As shown below in Table 24, about 53% of the energy in the mixed feed is derived from coal. The material balances for the coal gasifier were provided by AR; those for the POX reactor were estimated by GTI using Aspen Plus software. The operating conditions of the POX reactor were selected to match the flowrate as well composition of the syngas feed (Stream # 10 in Figure 18) to the FT reactor; this allows the production of the same amount of FT liquids (~9,609 BSD). The pressure and temperature at the POX reactor outlet are 800 psia and 2400 °F respectively. From the CO_2 recovery unit (located in the FT unit), pure CO_2 equivalent to ~32 vol% of the natural gas feed is recycled to the POX reactor to match the flowrate and composition of the fresh syngas feed to the FT reactor. The cost estimates include ~ 91% capture of the feed carbon in coal plus natural gas, and compression of captured CO_2 to ~2,200 psia. The DOE CTL Case captured 4,807 TPD CO_2 while the GTI C/GTL Case captured 3,411 TPD CO_2, about 30% less.

For the economic comparisons, we have assumed the annual capital-related expenses to be 13% of the total CAPEX which reflects ~12% ROI, and the annual OPEX-related expenses to be 9% of total CAPEX.

As shown in Table 29:

- The coal/natural gas option could reduce the cost of breakeven Brent crude price (BCP) by about 25% (based on a coal cost of \$1.70/MM Btu and \$4.00/MM Btu for natural gas); \$47/bbl for the coal/natural gas options vs. \$63 for the coal only option. If we take a 20 cents/gal credit for the zero-sulfur FT products, the BCP would be reduced to ~\$40/bbl and \$55/bbl respectively.
- The total CAPEX for the coal/natural gas option would be ~29% less than that projected by DOE for the coal-only case.

Comparative plant performance data and the power production/usage data for the two cases are compared in Table 25 and Table 26, respectively. The estimates on capital cost items for determining the total overnight capital cost (TOC) are compared in Table 27 and Table 28. provides more details on the capital cost differences between the DOE and GTI cases. Table 29 provides the key details on the annual O&M costs and the estimates on the Breakeven Crude Price with and without CO_2 TS&M.

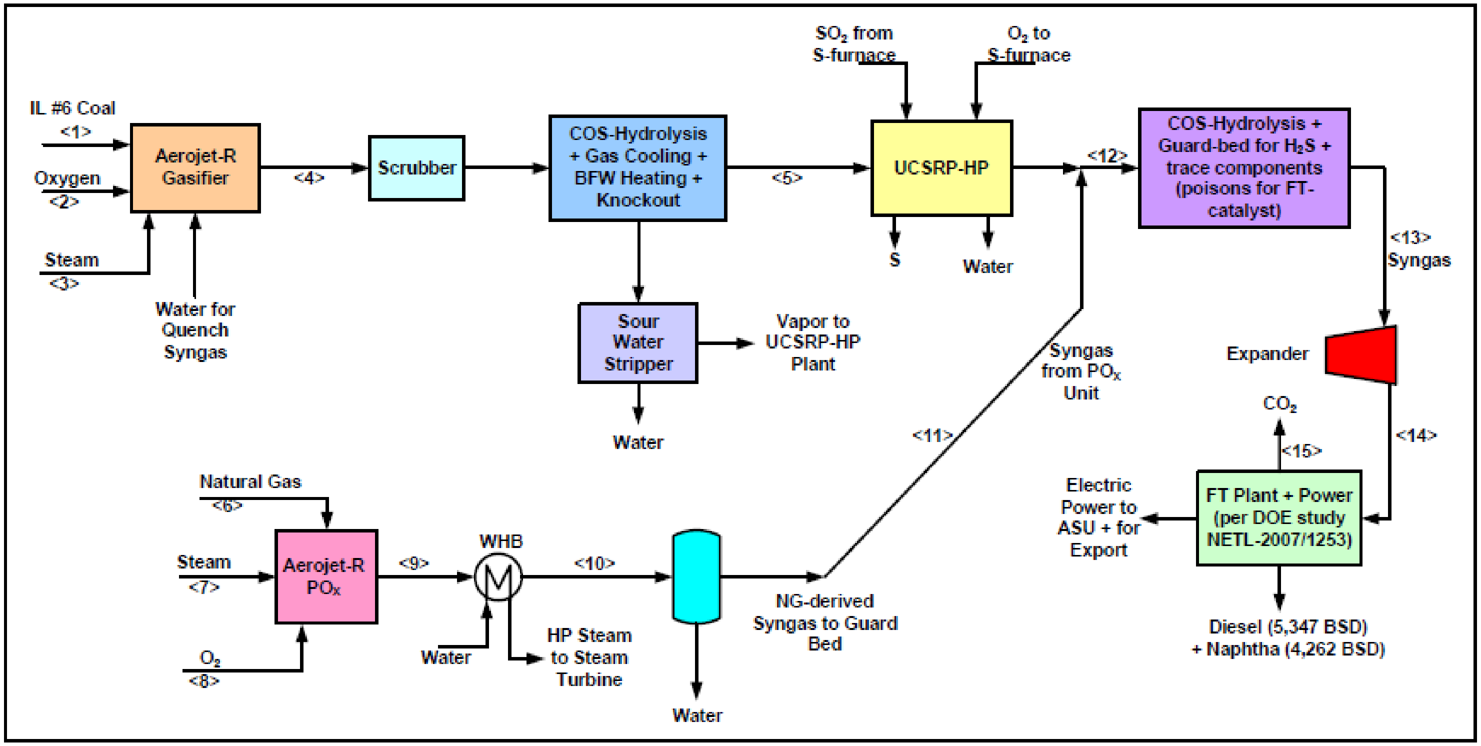


Figure 18 GTI C/GTL Base Case Flowsheet for the Production of Diesel and Naphtha from Coal and Natural Gas

Table 24 GTI C/GTL Case FT Production Plant Stream Data

Stream #	1	2	3	4	5	6	7
Description	Dry coal feed to AR Gasifier	Oxygen to AR Gasifier	Steam to AR Gasifier	Syngas from AR gasifier (after water-quench)	Coal-derived syngas to SR^2 (dry basis)	Natural gas Feed to POX	Steam to POX
Methane, mol%					0.0014	100.0	
H_2O			100	53.13	--		100.0
CO				28.17	60.26		
CO_2				4.33			
H_2				11.09	23.72		
O_2		99.5		--			
N_2		0.5		2.62	6.00		
COS ppmv				574	~0		
H_2S, ppmv				4,315	10,456	4	--
Ammonia				0.12	--		
HCl				0.05	--		
Pressure, psia	800+ psia to gasifier	800+	800+	~800	730	900	900
Temp., °F	ambient			proprietary	275	1,200	1,200
Kgmole/hr.	--	655.8	Proprietary	13,980	6,536.1	2,548.7	655.8
Kg/hr.	77,528	80,961	Proprietary	-		40,889	11814

Stream #	8	9	10	11	12	13	14	15	16
Description	Oxygen to POX Reactor	Syngas at POX Outlet	WHB Effluent	Near-dry syngas after HP separator	Blended syngas to Guard Beds	Clean syngas to Expander	Total CO_2 recovered from FT Plant	O_2 to SR^2 Unit	CO_2 Recycle to POX
Methane, mol%		0.02	0.02	0.03	0.02	0.02			
H_2O		19.60	19.6	0.18	0.1	0.1			
CO		31.69	31.69	39.36	49.43	49.43			
CO_2		5.20	5.20	6.43	7.85	7.85	100.0		100.0
H_2		43.40	43.40	53.89	39.89	39.89			
O_2	99.5	0.00	0.00	--	--	--		99.5	
N_2	0.5	0.09	0.09	0.11	2.71	2.71		0.5	
COS, ppmv					2	0			
H_2S, ppmv	--				4	0			
Ammonia						0			
HCl						0			
Pressure, psia	900	800	790	785	730	720			900
Temp., °F	572	2,400	100	100	100	112			1,200
Kgmole/hr.	1675.1	9,125.3	9125.3	7,347.9	13,815.8	13,815.7	4,049	34.3	819.7
Kg/hr.	53,570	142,348	142,348				178,197	1,097.8	36,075

Table 25 Comparative Process Data for FT Liquids Production

Design case	**DOE CTL Base Case**	**GTI C/GTL Case**
Plant Size (56 vol% diesel and naphtha), BSD	9,609	9,609
Coal feed rate (as received), TPD	3,859	1,961
Natural gas feed rate, TPD	--	981
% energy from coal	100	53
Oxygen need, TPD	3,565	3,313
H_2/CO molar ratio at coal gasifier scrubber exit	~0.80	~0.40
H_2/CO molar ratio for fresh syngas to FT reactor	~0.81	~0.81
Composition of Fresh syngas to FT reactor	Per DOE/NETL report # 2007-1253	Same as the DOE Case
CO_2 Recycle to POX reactor	Not applicable	Yes
CO_2 captured, TPD	4,807	3,411

Table 26 Plant Performance Summary for Liquid Products Production

	DOE CTL Base Case	GTI C/GTL Case	Units
Plant Output - 100 Percent Load			
Gas Turbine Power	34,330	34,330	kW_e
Steam Turbine Power	70,599	70,599	kW_e
Syngas Power Recovery Expander	8,197	8,197	
Steam Turbine Power from WHB in the POX Section	--	30,645	kW_e
Total	**113,126**	**143,771**	**kW_e**
Auxiliary Load Summary			
Coal Handling and Milling	1,710	710	kW_e
Coal Pump	400	650	kW_e
Slag Handling and Dewatering	850	150	kW_e
ASU Auxiliaries	--	1,000	kW_e
ASU Main Air Compressor	45,865	38,430	kW_e
Oxygen Compressor	8,935	9,300	kW_e
Fuel Gas Compressor	3,325	3,325	kW_e
All FT Processes	4,170	4,170	kW_e
BFW Pumps	875	875	kW_e
Flash Bottom Pump and Circulating water pump	1,490	1,800	kW_e
Scrubber Pump	203	200	kW_e
SR^2 and Sulfur/O_2 Furnace	--	1,000	kW_e
Recycle CO_2 Compressor to POX	--	910	kW_e
CO_2 Compression	6,325	4,475	kW_e
Steam Turbine Auxiliaries	--	300	kW_e
Transformer Losses	330	500	kW_e
Misc. BOP	3,000	3,000	kW_e
Selexol Plant Auxiliaries	1,976	--	kW_e
Claus Plant Auxiliaries	162	--	kW_e
Total	**79,616**	**70,795**	kW_e
Plant Performance			
Net Plant Power	-33,510	-72,976	kW_e
FT Liquids Production	9,609	9,609	bbl/d
As-received Coal Feed Flowrate	3,859	1,960	TPD
Natural Gas Flowrate	--	981	TPD

Table 27 Capital Cost Summary for Liquid Products Production

	DOE CTL Base Case	GTI C/GTL Case	Comment
Item/Description, $MM			
Coal Handling and Gasification	--	218.0	As-is IL #6 Coal Feed Rate = 1,960 TPD (Scale factor , SF, 0.6)
Coal/Sorbent Handling and Coal/water slurry Prep & Feed and Feed water & Misc. BOP Systems	79.9	--	
Gasifier & Accessories and Syngas Cooling and ASU and Misc. Gasification Equipment	415.9	--	
ASU	--	101.0	3,313 TPD Oxygen (SF : 0.35)
SR^2	--	4.0	To treat coal-derived syngas only
COS Hydrolysis and Scavenger Unit and Guard Beds (Post SR^2)	--	7.0	
Gas Cleanup (includes mercury removal, Selexol/Claus)	99.6	--	
Syngas Expander	--	11.0	9.2 MW_e output
FT Synthesis and Hydrocracking including CO_2 Removal	148.9	149.0	The cost is same as in the DOE CTL Base Case
Combustion Turbine Generator using FT Purge Gases	22.3	22.4	
HRSG/Ducting/Stack	8.3	8.3	
Steam Turbine and Associated units from FT Plant	26.0	26.0	Steam Turbine output : 70.599 MW_e
Cooling Water System	11.2	11.2	
Natural gas non-catalytic POX unit	--	9	Natural gas feed : ~51 MM SCF/day (Assume Pipeline Quality Gas @950 psia with ~4 ppmv H_2S
Natural gas/Steam/O_2 Preheaters for natural gas-POX	--	6	
WHB for syngas from natural gas-POX	--	21.0	HP Steam Generation : ~93.2 MW_{Th}
HP Separator after WHB		0.5	
Steam Turbine using HP-Steam from natural gas-POX WHB	--	20.0	Steam Turbine output : 30.7 MW_e
CO_2 Compression/Drying	--	17.0	CO_2 flow to Sequestration= ~141.9 metric tons/hr.
Replace the ATR unit in the FT plant by a POX unit	21.5	-$32	Net savings
Ash Handling		23.0	
Misc. Units	38.2	37.6	Accessory Electric Plant/Instruments/Site Improvement/Buildings (5+11.6+11+10 MM)
TOTAL PLANT CAPEX	**927**	**660**	

Table 28 Key Capital Cost Differential for Liquids Production

Units	DOE CTL Base Case	GTI C/GTL Case	CAPEX Savings
Coal Gasification and ASU	495	--	
Gasification and POX and WHB and Preheaters and ASU and Recycle CO_2 Compressor	--	355	140
Syngas cleanup, Single-stage Selexol/Claus (no CO_2 capture) and Expander vs. SR^2/COS-hydro./Guard-beds/Expander	113	22	91
Ash handling, Misc. units (e.g., process control), CO_2 Compression	102	81	21
Eliminate ATR unit in the FT Plant with POX		-35	-35
Add Steam turbine for natural gas-POX unit		19	19
Total Differential, $MM	**-**	**-**	**268**

Table 29 Liquid Products Production Costs

Design Case	DOE CTL Base Case	GTI C/GTL Case	Units
Total CAPEX	928	669	$MM
Power generation	113.126	143.771	MWe
Total auxiliary load	73.598	70.795	MWe
Import (export) of electricity	(33.204)	(85.914)	MWe
Annual CAPEX plus OPEX costs @ 22% of Total CAPEX	204.2	145.0	$MM/yr.
Export of Electricity,	33.2	73.0	MW_e
Credit @10 cents/kWhr	26.2	57.6	$MM/yr.
Total credits (with no credit for zero-sulfur liquids)	26.2	57.6	$MM/yr.
Net Costs	234.8	177.6	$MM/yr.
Required Selling Price (RSP) at the Plant Gate	74.4	56.2	$/bbl
Breakeven Crude Price (BCP : RSP x 0.84)	62.5	47.2	$/bbl
BCP with an additional 20 cents/gal credit for zero-sulfur FT Liquids	55.4	40.2	$/bbl

CONCLUSIONS AND RECOMMENDATIONS

Conclusions reached in this project are:

- Achieved >90% H_2S conversion with outlet H_2S concentration of less than 8 ppmv in the SR^2 unit. Costs were included to remove sulfur emissions to less than 1 ppb for all cases studied.
- The SR^2 unit can achieve 80-90% ammonia and chloride removal.
- SR^2 ready for pilot testing and further scale up.
- Utilization of natural gas with coal was found to be favorable for each of the three cases studied in this project. Product costs were reduced by 5-30% over the base line coal only plants, even with the annual fuel costs for the GTI cases up to 70% higher than the DOE case due to the cost differences between coal at \$1.70/MM Btu and natural gas at \$4.00/MM Btu.
- Natural gas POX operates at a much higher outlet temperature than achievable with coal gasification. This allows for significant heat recovery via WHB and hence greater electricity production.
- The GTI cases produced 18-30% less CO_2, reducing the sequestration load on the environment.
- Using overall energy input of 51% coal in the Advanced Compact gasifier and 49% natural gas in a non-catalytic POX for a plant producing ~500 MW_e with GTI's SR^2 process for sulfur removal, the GTI IGCC Case could reduce the cost of electricity production by about 5%, and the total CAPEX would be reduced by ~20% as compared with DOE IGCC Case reported in DOE/NETL Report # 2015/1727. For an IGCC plant with the carbon capture case, the GTI process showed savings in CAPEX but higher OPEX resulting in a reduction in LCOE.
    - The estimated Levelized Costs of Electricity, including CO_2 TS&M are \$127/MW_e for the GTI case vs. \$134/MW_e for the DOE coal only case.
- Using overall energy input of 51% coal in the Advanced Compact gasifier and 49% natural gas in a non-catalytic POX for a plant producing ~650 TPD of 99.9% pure chemical-grade hydrogen with GTI's SR^2 process for sulfur removal, the GTI Hydrogen Case could reduce the cost of hydrogen production by about 20%, and the Total CAPEX would be reduced by ~31% as compared with DOE Hydrogen Case reported in DOE/NETL Report # 2010/1434.
    - The estimated first year hydrogen production cost, including CO_2 TS&M are \$2.71/kg for the GTI case vs. \$3.71/kg for the DOE coal only case.
- Using overall energy input of 53% coal in the Advanced Compact gasifier and 47% natural gas in a non-catalytic POX for a plant producing ~9,609 BSD of diesel and naphtha at ~56 vol. % diesel with GTI's SR^2 process for sulfur removal, the GTI C/GTL Case could reduce the cost of breakeven Brent Crude Price (BCP) by about 30%, and the total CAPEX would be reduced by ~29% as compared with DOE CTL Case reported in DOE/NETL

Report # 2007/1253.

  - Breakeven Brent Crude prices are \$47/bbl for the GTI Case vs. \$63/bbl for the DOE Case
  - If a 20 cents/gallon credit is allowed for zero-sulfur FT liquids, GTI Case BCP = \$40/bbl vs \$55/bbl for the DOE Case

- PBI supports synthesized during this project were not acceptable for hydrogen selective membranes; there was evidence that their pore sizes were inconsistent and that they were not stable at the high temperatures that were required for the metals to be hydrogen permeable.
- Metal layers were successfully coated on the polymers using a sputtering process. Synthesized membranes show complete impermeability most likely due to vanadium oxide layer formation when the membrane was exposed to air.
- If a membrane could be developed that meets DOE 2015 Targets for Hydrogen Membranes [6], further savings could be achieved in the capital and operating costs for the hydrogen and IGCC cases.

For further scale up of the SR^2 process, we recommend future experimental programs to:

- Conduct pilot scale testing at gas flow rate up to 1 MMSCFD.
- Use a down-flow co-current reactor, fitted with SMV packing, with a larger internal diameter to study various reactor scale-up parameters.
- Test the process with syngas from an operating coal gasifier using Illinois #6 coal to see if there are any changes to: H_2S conversion due to presence of syngas components as well as CO_2 and removal of NH_3 and HCl if the two components are present in a gas stream at the same time in the presence of water as well as other contaminants like mercury, selenium and arsine.
- Extend the operating pressures to ~800-1000 psig.
- Explore, if other solvents, e.g., the Uhde/GTI Morphysorb® or dimethylether of polyethylene glycol (generic Selexol), can be used as the solvent in the SR^2 process. If confirmed, this would avoid process complications related to mixing of DGM solvent with that used in the downstream CO_2-removal step.

For further hydrogen membrane development we recommend experimental programs to:

- Explore other support materials, such as ceramics, metallic fibers and sintered metals.
- Explore different metals/alloys, such Nb, Ta etc.
- Explore other deposition methods.
- TEA can be refined to get values that are more accurate after SR2 pilot testing and when the membrane development program is successful.

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1. DOE/NETL-2007/1253, “Technical & Economic Assessment of Small-Scale Fischer Tropsch Liquids Facilities”, Feb. 27, 2007.
2. DOE/NETL-401/062006, “Comparison of Pratt and Whitney Rocketdyne IGCC and Commercial IGCC Performance”, final report, June 2006.
3. DOE/NETL-2015/1727, “Cost and Performance Baseline for Fossil Energy Plants, Volume 1b: Bituminous Coal (IGCC) to Electricity”, revision 2b-Year Dollar Update, July 31, 2015.
4. "Economic Evaluation of the UCSRP-HP Process in IGCC Applications", Arunabha Basu, Ajay Makkuni, S. James Zhou, Howard S. Meyer, International Journal of Clean Coal and Energy, Vol.2 No.3, 2013.
5. DOE/NETL-2010/1434, “Assessment of Hydrogen Production with CO_2 Capture, Volume 1: Baseline State-of-the-Art Plants”, August 30, 2010.
6. DOE/NETL-2008/1335, “NETL Testing Protocol – Testing of Hydrogen Separation Membranes”, October 2008.
   - **2015 Target**
     − Hydrogen flux – 300 SCFH/ft^2 (~ 150 sccm/cm^2) @ 100 psi ΔP H_2 partial pressure. Standard conditions are 150 psia hydrogen feed pressure and 50 psia hydrogen sweep pressure.
     − Temperature – 250 to 500 °C (482 to 932 °F).
     − Pressure performance – ΔP – 800 to 1000 psi.
     − Sulfur tolerance – >100 ppm.
     − CO tolerance – Yes.
     − WGS activity – Yes.
     − Hydrogen purity – 99.99 %.
7. “Partial Oxidation Gas-Turbine Based TURBO-POx Syngas Generation Technology for GTL Applications”, Basu, A. and Fusselman, S. Presented at GTL Technology Forum 2014, Houston TX (July 30, 2014) based on work performed under Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy (DOE), under Award Number DE-AR0000290. (http://www.gulfpub.com/product.asp?PositionID=&ProductID=19071)

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APPENDIX A

GENERAL EVALUATION BASIS

Site Description

The generic characteristics for the plant sites are presented in Table 30 and Table 31.

Table 30 Site Ambient Conditions

Elevation, ft	0
Barometric Pressure, psia	14.696
Design Ambient Temperature, Dry Bulb, °F	59
Design Ambient Temperature, Wet Bulb, °F	51.5
Design Ambient Relative Humidity, %	60

Table 31 Site Characteristics

Location	Greenfield, Midwestern USA
Topography	Level
Size, acres	300
Transportation	Rail (GTI), Road, Rail, Barge, Pipeline (DOE)
Ash/Slag Disposal	Off Site
Water	Municipal (50%) / Groundwater (50%), River (DOE)
Access	Land locked, having access by rail and highway
CO_2 Storage	Compressed to 15.3 MPa (2,215 psia), transported 50 miles and sequestered in a saline formation at a depth of 1,239 m (4,055 ft)

The following design parameters are considered site-specific, and are not quantified in this study. Allowances for normal conditions and construction requirements, however, will be 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

Design Fuel Characteristics

The design coal is Illinois No. 6 with characteristics presented in Table 32. The coal properties are from NETL's Coal Quality Guidelines. The coal cost used in this study is

$1.70/MMBtu, which is presented as delivered cost of coal to electric utilities in 2013 dollars.

Table 32 Design Coal Characteristics

Rank	**Bituminous**	
Seam	**Illinois No. 6 (Herrin)**	
Source	**Old Ben Mine**	
Proximate Analysis (weight %)		
	As Received	**Dry**
Moisture	11.12	0.00
Ash	9.70	10.91
Volatile Matter	34.99	39.37
Fixed Carbon	44.19	49.72
HHV, Btu/lb	11,666	13,126
HHV, kJ/kg	27,113	30,506
LHV, Btu/lb	11,252	12,712
LHV, kJ/kg	26,151	29,544
Ultimate Analysis (weight %)		
	As Received	**Dry**
Moisture	11.12	0.00
Carbon	63.75	71.72
Hydrogen	4.50	5.06
Nitrogen	1.25	1.41
Chloride	0.29	0.33
Sulfur	2.51	2.82
Ash	9.70	10.91
Oxygen	6.88	7.75
Total	100.00	100.00

The design natural gas is utilized as another fuel in GTI cases and its composition is presented in Table 33. The cost of natural gas used in this study is $4.00/MMBtu, which is presented as delivered cost of natural gas to electric utilities in 2013 dollars.

Table 33 Natural Gas Characteristics

Component	Volume Percentage	
Methane	CH_4	93.1
Ethane	C_2H_6	3.2
Propane	C_3H_8	0.7
n-Butane	C_4H_{10}	0.4
Carbon Dioxide	CO_2	1.0
Nitrogen	N_2	1.6
Total		100.0
	LHV	**HHV**
kJ/kg	47,454	52,581
MJ/scm	34.71	38.46
Btu/lb	20,410	22,600
Btu/scf	932	1,032

Environmental Requirements

The environmental control equipment used in the conceptual design conforms to Best Available Control Technology (BACT) guidelines. Specific emission limits and the corresponding environmental control equipment are summarized in Table 34.

Table 34 BACT Guidelines

Gasification Technologies		
Pollutant	**Control Technology**	**Limit**
Sulfur	SR^2 (GTI) Selexol/Econamine Plus/Sulfinol-M and Claus Plant (DOE)	99+% or ≤ 0.050 lb/10^6Btu
NOx	Low-NOx Burners and N_2 Dilution	15 ppmvd (@ 15% O_2)
PM	Cyclone/Barrier Filter/Wet Scrubber/AGR Absorber	0.006 lb/10^6 Btu
Hg	SR^2 (GTI) Activated Carbon Bed (DOE)	95% removal

Carbon Dioxide

Carbon dioxide emissions from the plant are captured and prepared for transportation as a supercritical stream for sequestration. Nominally 90% of the plant CO_2 is captured and compressed to 2,200 psia.

Mercury

The GTI plant designs assume >95% mercury is captured via SR^2, based on laboratory data collected by GTI with simulated coal-derived syngas. The DOE plant designs assume mercury capture of 95% via activated carbon, based on data from the Eastman Chemical

Company's gasification facility in Kingsport, Tennessee. EPA has determined that some mercury is captured in systems conventionally used to capture PM, sulfur, and nitrogen oxides. Oxidized mercury is captured in fabric filters and electrostatic precipitators, wet and dry flue gas desulfurization (FGD) systems, and selective catalytic reduction and selective non-catalytic reduction (SCR/SNCR) systems. The co-benefit of mercury capture in these systems is particularly high for bituminous coals, ranging from 84 to 98%. The analysis estimates co-benefit mercury capture and factors the result into the design of the activated carbon mercury control system.