

1. INTRODUCTION

1.1 BACKGROUND

In 1999, both Parsons Infrastructure & Technology Group (Parsons) and the National Renewable Energy Laboratory (NREL) prepared conceptual plant designs and cost estimates for producing hydrogen from coal gasification. Parsons' approach to producing hydrogen focused on integrating high-temperature ceramic membranes with coal gasification to both shift and separate hydrogen from the syngas.³ Parsons also prepared a base case design for hydrogen from coal gasification utilizing conventional technology. This included a Wabash River-scale Destec gasifier, conventional gas cooling, commercial acid gas cleanup, commercial sulfuric acid technology, and commercial pressure swing adsorption.

The NREL approach to plant design focused on advanced and conventional technology for hydrogen production with high-temperature gas cleanup, shift, and pressure swing adsorption (PSA) purification, augmented with various concepts to sequester carbon dioxide (CO₂) and increase hydrogen production.⁴ These concepts consisted of a base case design for production of hydrogen from coal gasification accompanied by CO₂ sequestration in coal seams, reforming extracted methane, and producing power from extracted coal seam methane. The base case cost for producing hydrogen from coal gasification was reported by Parsons to be \$5.57/MMBtu, while NREL reported the base case cost for hydrogen from coal gasification to be \$18.97/MMBtu.

1.1.1 Plant Configurations

Comparing the two base case plants, there are numerous differences. One difference between the plant designs had to do with the selection of coal. Parsons used Pittsburgh No. 8, while NREL used Wyodak PRB (Powder River Basin). The plants have the Destec gasifier in common, followed by quench and cooling with a fire-tube boiler heat exchanger. The single Destec gasifiers handled similar mass throughputs, and hydrogen production per thermal input is similar. However, the Wyodak coal resulted in less hydrogen production due to its lower heating value. The gas from both plants is cleaned of particulate with a metallic or ceramic filter at about 600°F.

To remove H₂S from the gas prior to the carbon monoxide (CO) shift reaction, NREL uses an advanced DOE hot gas desulfurization process. The sulfur dioxide (SO₂) released from regeneration of the sorbent is sent to a sulfuric acid plant. The desulfurized gas is sent to the high- and low-temperature shift reactors.

³ "Decarbonized Fuel Production Facilities/Base Case Comparisons," Letter Report, U.S. DOE, June 1999.

⁴ Spath, Pamela and Amos, Wade, "Technoeconomic Analysis of Hydrogen Production from Low-Btu Western Coal Augmented with CO₂ Sequestration and Coalbed Methane Recovery Including Delivered Hydrogen Costs," NREL, September 1999.

By using a sulfur-tolerant catalyst, as in the Parsons plant, the CO shift reaction can occur directly following the syngas cooler and filter. The hydrogen sulfide (H₂S) and most of the remaining CO₂ following the shift can be removed at low temperature. Haldor Topsoe and others⁵ have indicated that they offer sulfur-tolerant shift catalysts for which the presence of H₂S is actually beneficial to maintaining catalyst activity. The Parsons plant design uses a staged Selexol acid gas removal (AGR) process following the sour shift. This results in separate CO₂ and H₂S streams. The CO₂ is recovered at low pressure, and the H₂S is fed to a sulfuric acid plant.

Parsons uses the combined sources of steam from the plant cooling for generation of power with steam turbines, and the low-pressure steam is used for regeneration of the AGR process. To achieve maximum CO₂ recovery, the retinate gas from the PSA can be fired in a heat recovery steam generator (HRSG) with oxygen to produce steam for power and a clean recoverable CO₂ stream in the stack.

Table 1-1 lists the differences and common features in the two designs.

**Table 1-1
Comparison of Parsons and NREL Plants**

	Differing		Common
	Parsons	NREL	
Coal	Pittsburgh No. 8	PRB Wyodak	
Gasifier			Destec
Gas Cleanup	Cold	Hot	
ASU			Conventional cryogenic
Acid Gas Removal	Selexol	Hot zinc titanate	
Sulfur Product			Sulfuric acid
Water Gas Shift	Sour gas high temperature	Clean gas, high and low temperature	
Hydrogen Purification			PSA
Excess Steam	Used to make power	Shipped off-site	
PSA Off-Gas	Fired in HRSG with oxygen to maximize CO ₂	Treated as CO ₂ and used for coal bed methane	
Captured CO ₂	Pure stream sent off-site	Coal bed methane	

⁵ Rasmussen, H.W. and Houken, J., "Topsoe Hydrogen Plant Catalysts with Focus on Industrial Experience and Solutions to Operational Problems," Haldor Topsoe Refining Seminar, San Antonio, Texas, September 17-19, 1997.

1.1.2 Summary of Plant Differences

As shown in Table 1-2, the overall equivalent efficiency of the NREL plant differs from the Parsons plant due to the value of steam and PSA off-gas being credited in the numerator as a byproduct. Parsons used available energy streams to produce electricity, resulting in a lower equivalent efficiency.

**Table 1-2
Performance Summary**

Parameter	Parsons	NREL	Significant Differences
Coal Feed	221,631 lb/h	249,764 lb/h	
Thermal Input	2,759 MMBtu/h	2,155 MMBtu/h	
Oxygen Feed (95%)	178,860 lb/h	NOT REPORTED	
Hydrogen Product	26,487 lb/h	17,645 lb/h	
Sulfuric Acid Byproduct	19,100 lb/h	2,598 lb/h	Parsons has a larger H ₂ SO ₄ plant due to higher sulfur in coal
Gross Power Production	77 MW	NOT REPORTED	
Auxiliary Power Requirement	41 MW	NOT REPORTED	
Net Power Production	36 MW	12 MW	Parsons produces more power
Equivalent Plant Efficiency, HHV	63.1%	83.0%	NREL takes credit for fuel value of PSA off-gas

1.1.3 Financial Assumptions and Cost Data

The differences in financial assumptions as shown in Table 1-3 should be recognized as being unique to the project for which the respective studies were conducted. Similar assumptions would lead to similar results.

**Table 1-3
Financial Assumptions**

Parameter	Parsons	NREL
Capacity Factor	95%	90%
Excess Steam Usage	Make power	Sell off-site
Coal Cost	\$1.00/MMBtu	\$0.82/MMBtu
Electricity Revenue	\$30.00/MWh	\$50.00/MWh
Debt/Equity	80/20	0/100
Cost of Debt	6.3%	N/A
Return on Equity	16.5%	15%
Book Life	30 years	20 years

1.1.4 Capital and Operating Costs

The primary differences in the cost of hydrogen from the Parsons and NREL plants can be realized from the Total Plant Investment (TPI) as shown in Table 1-4. The TPI for the NREL plant per unit of hydrogen production is 2.3 times that of the Parsons plant.

**Table 1-4
Capital and Operating Cost Comparison**

Parameter	Parsons	NREL	Significant Differences
Total Plant Cost	\$374 million ('97)	NOT REPORTED	
Total Plant Investment	\$398 million ('97)	\$612 million ('95)	Significantly higher for comparable-sized plant
Cost/lbH ₂ /h	\$15,026/lb/h	\$34,684/lb/h	2.3x higher
Cost/scfd	\$3.49/scfd	\$8.05/scfd	2.3x higher
Annual Coal Cost	\$22.960 million	\$13.93 million	
Annual O&M	\$12.836 million	17 million	
Annual Credits	(\$14.963 million)	(\$5.289 million)	
Steam Credit	None	NOT REPORTED	

1.1.5 The Need for Reconciliation of Cost Estimates

Due to the wide differences in reported costs for capital and the need to provide a baseline cost for hydrogen production, NETL has tasked Parsons to review its prior plant design and cost estimate for producing hydrogen from coal gasification. To arrive at a cost estimate for hydrogen based on reliable information that is acceptable throughout DOE, a design will be prepared using commercially available process technology, supplied by vendor sources that can provide quotations based on direct experience.

The key benefit of utilizing commercial technology is the obtaining of credible cost estimates for the plant, with a minimum of process contingency. The results of this effort are intended to prepare a basis from which to utilize individualized financial parameters in the DOE IGCC Cost Estimating Model to arrive at a selling price for hydrogen.

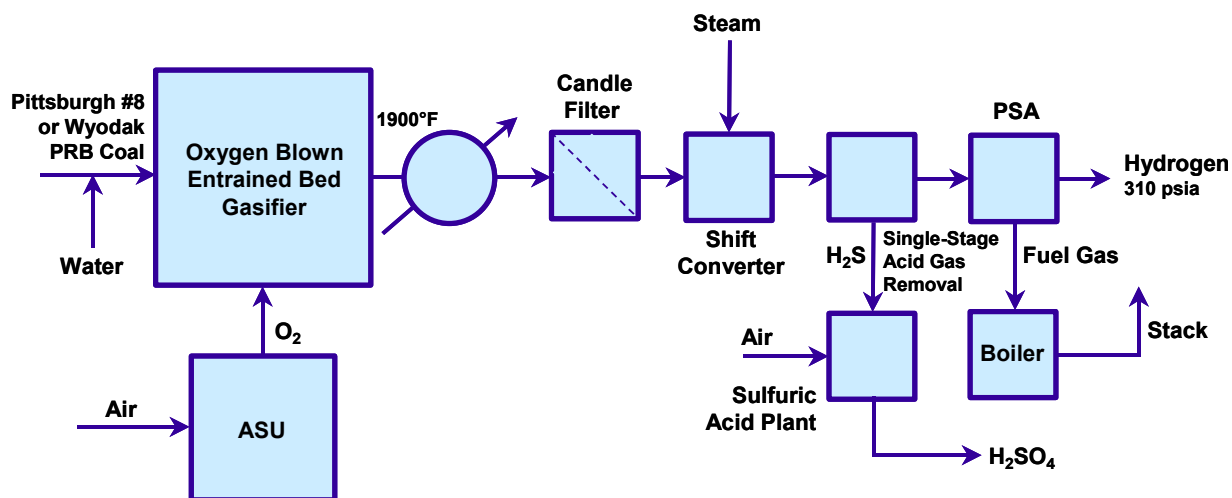
Focus of the plant design will be from a common thermal gasifier throughput. Two coals will be reviewed, Pittsburgh No. 8 and Wyodak PRB. Hydrogen costs from these coals will be prepared to quantify the differing plant characteristics associated with bituminous coal or sub-bituminous coal. Plant design areas common to each coal will be defined, but may be of different size due to coal selection.

1.2 TASK OBJECTIVE

The objective of this task was to prepare capital and operating cost data to be used to arrive at a plant gate cost for hydrogen produced from coal gasification. The two coals used in this study are Pittsburgh No. 8 bituminous and Wyodak PRB sub-bituminous. Hydrogen cost was determined by first preparing two plant designs for hydrogen production, based on currently available process technology, and meeting current permitting regulations for environmental compliance. These baseline plants will not capture CO₂.

To arrive at a cost estimate for hydrogen, the design included commercially available process technology obtained from verifiable sources. The plants utilized commercially available technology including a Wabash River-scale Destec (E-Gas™) gasifier, conventional gas cooling, commercial shift conversion and acid gas cleanup, commercial sulfuric acid technology, and commercial PSA. The E-Gas™ gasifier is the gasifier of choice for this study since it has been operated on both bituminous and sub-bituminous coals. Figure 1-1 is the block flow diagram for the plant.

Figure 1-1
Block Flow Diagram
Conventional Hydrogen Plant



The E-Gas™ gasifier is used to partially react a coal/water slurry with oxygen at high pressure. Gas exiting the gasifier is cooled in a fire-tube boiler to 625°F and cleaned of particulate matter. Particulates are recycled to the gasifier. Steam is added to the raw syngas, which passes through a reactor containing high-temperature sulfur-tolerant CO shift catalyst for conversion of the CO and steam to hydrogen and CO₂. The syngas containing predominantly hydrogen and CO₂ is cooled to less than 105°F and enters the AGR process. H₂S is removed and recovered for conversion to sulfuric acid. The remaining syngas goes through a PSA process to produce pure hydrogen at pressure. The PSA offgas is fired in an auxiliary boiler.

The plant design and cost estimates are addressed in two separate sections: Pittsburgh No. 8 bituminous coal and Wyodak PRB sub-bituminous coal. Sections 1.4 and 1.5 include the rationale for process selection and the basis for determining installed costs of the major process areas, respectively. Each section of this report contains a heat and material balance, process description with process flow diagram and stream composition tables, and a list of major equipment. Each section also presents the capital and operating costs and a calculated cost of hydrogen, based on preliminary economic assumptions. These hydrogen values are used in the final section, wherein the U.S. DOE integrated gasification combined cycle (IGCC) financial model is used to calculate the internal rate of return (IRR) for both coal cases.

1.3 PLANT DESIGN BASIS

1.3.1 Plant Capacity and Availability

The overall availability of the operating plant will be 90 percent. This is a high factor for single train gasification, and will result in two gasifier trains, operating at 50 percent capacity with the capability to ramp up to 100 percent. The balance of plant will be single train, operating at 100 percent capacity, based on commercial process operating experience as verified by equipment vendors.

Product Specifications:

- Sulfur as 98 percent pure H₂SO₄
- Hydrogen: 99 percent pure, 300 psig

Coal Properties:

- Pittsburgh No. 8; see Table 1-5.
- Wyodak PRB; see Table 1-6.

**Table 1-5
Coal Analysis – Pittsburgh No. 8**

Ultimate Analysis			
Constituent	Air Dry, %	Dry, %	As Received, %
Carbon	71.88	73.79	69.36
Hydrogen	4.97	4.81	5.18
Nitrogen	1.26	1.29	1.22
Sulfur	2.99	3.07	2.89
Ash	10.30	10.57	9.94
Oxygen	8.60	6.47	11.41
Total	100.00	100.00	100.00
Proximate			
		Dry Basis, %	As Received, %
Moisture		--	6.00
Ash		10.57	9.94
Volatile Matter		38.20	35.91
Fixed Carbon		51.23	48.15
Total		100.00	100.00
Sulfur		3.07	2.89
Btu Content		13,244	12,450
Moisture and Ash Free (MAF), Btu		14,810	
Ash Analysis, %			
Silica, SiO ₂		48.1	
Aluminum Oxide, Al ₂ O ₃		22.3	
Iron Oxide, Fe ₂ O ₃		24.2	
Titanium Dioxide, TiO ₂		1.3	
Calcium Oxide, CaO		1.3	
Magnesium Oxide, MgO		0.6	
Sodium Oxide, Na ₂ O		0.3	
Potassium Oxide, K ₂ O		1.5	
Sulfur Trioxide, SO ₃		0.8	
Phosphorous Pentoxide, P ₂ O ₅		0.1	
Total		100	
Ash Fusion Temperature			
		Reducing Atmosphere, °F	Oxidizing Atmosphere, °F
Initial Deformation		2015	2570
Spherical		2135	2614
Hemispherical		2225	2628
Fluid		2450	2685

**Table 1-6
Wyodak Coal Properties**

Proximate	As Received Basis	Dry Basis
Moisture	26.6	0
Volatile Matter	33.2	45.23
Fixed Carbon	34.4	46.87
Ash	5.8	7.90
Ultimate		
Sulfur	0.6	0.82
Hydrogen	6.5	4.82
Carbon	50.0	68.12
Nitrogen	0.9	1.23
Oxygen	36.2	17.11
Ash	5.8	7.90
Heating Value, HHV	8,630 Btu/lb	11,757 Btu/lb

Table 1-7 lists the plant design criteria and site conditions.

**Table 1-7
Design Criteria for Conventional Hydrogen Production Plant**

Hydrogen Production Plant Parameter	Hydrogen Production Plant Design Basis
Ambient Conditions	14.7 psia, 60°F, river water access
Coal Feed	Pittsburgh No. 8/PRB Wyodak
Gasifier	Oxygen-blown E-Gas™ with second stage adjusted for 1900°F output
Coal Feed Rate	2,500 tpd dry basis
Hot Gas Temperature	~1900°F
Gasifier Outlet Pressure	450 psia
Gas Quench/Cooling	625°F
Metallic Candle Filter	Following quench/cooling
CO-Shift	Single-stage high-temperature, sulfur-tolerant
Desulfurization	Proprietary amine
Sulfur Recovery	Sulfuric acid byproduct
CO ₂ Recovery	None
Hydrogen Purification	Pressure swing adsorption
PSA Retinate Gas	Fired in auxiliary boiler
CO ₂ Product Pressure	N/A
Hydrogen Utilization	315 psia at plant gate
Auxiliary Power Block	Steam turbine generator
Plant Size	Maximum hydrogen production from 2,500 tpd dry coal feed
Plant Capacity Factor	90 percent

1.4 PROCESS SELECTION

1.4.1 Gasifier

The E-Gas™ gasifier is selected for these plants because of the wide differences in the coals to be compared. The E-Gas™ two-stage design has resulted in successful operation on both bituminous and sub-bituminous coals. By comparison, the Texaco gasifier with its single-stage entrained slurry feed reaches operational limitations with high-moisture coals, e.g., sub-bituminous and lignite.

1.4.2 Shift Reactor Catalyst

For the conversion of the gasifier product to hydrogen, the first step is to convert most of the CO to hydrogen and CO₂ by reacting the CO with water over a bed of catalysts. This produces approximately 45 percent of the gross hydrogen product and converts more than 80 percent of the carbon monoxide to hydrogen and CO₂. The CO shift converter can be located either upstream of the AGR or immediately downstream. If the CO converter is located downstream of the AGR, then the metallurgy of the unit will be less stringent, but additional equipment must be added to the process. Products from the gasifier will be steam-injected to reach sufficient amounts of water vapor to meet the necessary water to gas criteria at the reactor inlet. If the CO converter is located downstream of the AGR, then the gasifier product would first have to be cooled and the free water separated and treated. Additional steam would have to be generated and reinjected into the CO converter feed to meet the required water-to-gas ratio. If the CO converter is located upstream of the AGR step, no additional equipment is required. Therefore, for this plant design the CO converter was located upstream of the AGR unit.

The CO shift catalyst selected for these plants is the Haldor-Topsoe SSK Sulfur Tolerant CO Conversion Catalyst. The plant will utilize a single-stage high-temperature shift, resulting in a CO conversion of greater than 80 percent. The SSK catalyst also promotes carbonyl sulfide (COS) hydrolysis, thereby resulting in an acid gas consisting of all H₂S.

1.4.3 Acid Gas Removal

The traditional approach to acid gas removal is with regenerable amines. Other methods include removal of H₂S with membranes systems or with molecular sieves. Regenerable amines are by far the most popular means of removal of acid gas from all types of gaseous streams.

Acid Gas Removal with Amines. The amine solvents are typically categorized into chemical, physical, and hybrid solvents. Hybrid solvents can be described as weak chemical solvents. The general flow scheme is similar for all of these solvents, and the choice depends on criteria such as AGR requirements, selectivity for H₂S compared to CO₂, organic sulfur removal requirements, regeneration energy requirements, and the presence of heavy hydrocarbons.

Chemical solvents remove CO₂ along with the H₂S. Examples of chemical solvents are monoethanolamine (MEA), diethanolamine (DEA), and diglycolamine (DGA).

Physical solvents are proprietary solvents that are selective toward H₂S and achieve the removal by equilibrium effects due to the more favorable solubility of H₂S. In order to achieve the solubility effect, refrigeration of the solution or compression and recycle is normally required, which increases the capital investment.

Hybrid solvents have removal capabilities between the chemical and physical solvents. The most common hybrid solvent is methy-diethanolamine (MDEA), which is a tertiary amine. In addition to MDEA, other hybrid solvents include diisopropanolamine (DIPA) and specialty amines such as Exxon's FLEXSORB, Union Carbide's UCARSOL HS solvents, and Dow Chemical's GAS/SPEC SS Solvent. FLEXSORB solvent is described as a severely sterically hindered amine and is the most selective for H₂S of any solvent currently marketed.

Acid Gas Removal with Membranes. Cellulose acetate membranes have been used successfully for acid gas pretreatment in gas processing facilities. Membranes are typically used for pretreatment of natural gas streams upstream of an amine unit. However, since the permeation rate for H₂S is similar to that of CO₂, membranes are not suitable for selective removal of H₂S.

Acid Gas Removal with Molecular Sieves. Molecular sieves have a large surface area in addition to highly localized polar charges and can be used for selective removal of H₂S. A type 5A molecular sieve is typically used for this type of application. One problem with the use of molecular sieves for H₂S removal is that the alumina in the molecular sieve catalyzes the formation of COS from H₂S and CO₂.

The basic criteria for selecting the technology were selective removal of H₂S, ease of operation, and a single type of system. Chemical absorption, e.g., MEA, MDEA proprietary amines, operates at lower pressure, and removes both CO₂ and H₂S. Therefore, the AGR process selected for these plants is a proprietary amine with an H₂S concentrator on the regenerated acid gas. The gas from the AGR process, concentrated in H₂S, will be used as a feed for a Monsanto H₂S-fired sulfuric acid plant.

1.4.4 Hydrogen Purification

The three main processes for hydrogen purification are the pressure swing adsorption, the selective permeation process using polymer membranes, and the cryogenic separation process. Each of these processes is based on a different separation principle, and the process characteristics differ significantly.

Pressure Swing Adsorption. The PSA units are based on the capacity of adsorbents to adsorb more impurities at high gas partial pressure than at low gas partial pressure.

These systems are the most commonly used. Two advantages of the PSA process are its ability to remove the very undesirable impurities down to a low level and to produce a very high purity hydrogen product. Typically, hydrogen product purities range from 99 to 99.999 vol %, and removal of CO and CO₂ to less than 10 ppmv is easily achieved. The amount of hydrogen recovered is dependent on inlet pressure, purge gas pressure, level of impurities, and hydrogen concentration. Hydrogen recovery with the feed gas produced for this project should be approximately 85 percent.

Polymer Membranes. Selective permeation through polymer membranes is a relatively recent and rapidly evolving commercial separation development. The process is based on the difference in permeation rates between hydrogen and impurities. Gas phase components must first dissolve into the membrane, then diffuse through it to the permeate side. For a hydrogen recovery membrane system, the very high hydrogen purity is not practical as the recovery of hydrogen falls rapidly as the purity goes up. For example, an increase in hydrogen purity from 95 to 98 percent will result in greater than a 25 percent decrease in hydrogen recovery.

Cryogenic Process. The cryogenic process is a low temperature separation process, which uses the difference in boiling temperatures of the feed components to effect the separation. Hydrogen has a high relative volatility compared to hydrocarbons. However, if the feed contains significant amounts of CO and CO₂ such as the feed in this project, a methane wash column is required. This column is used to wash the impurities from the hydrogen product stream, which is necessary to reduce CO and CO₂ to the low levels required. Also, because of the water in the feed stream, a drying system would have to be added upstream of the cryogenic system. Higher hydrogen recovery at moderate hydrogen purities (95 percent or less) is possible with a cryogenic system; however, very high hydrogen purity is not practical. Because of the type and composition of the feed gas, a cryogenic system is not acceptable.

The PSA system was selected based on the ability to produce high purity (99.9 percent) hydrogen, low amounts of CO and CO₂, ease of operation, and a single system.

1.5 APPROACH TO COST ESTIMATING

1.5.1 Gasifier

The gasifier specified for production of H₂ was the E-Gas™ gasifier. The cost in the evaluation was based on the reported cost of the E-Gas™ gasifier in the IGCC Reference Plant, E-Gas™, Final Report, dated February 2002. The same cost basis was utilized. In this evaluation, compared to the reference cost, two trains of gasifier were utilized to increase availability to 90 percent. The cost for the syngas cooling was adjusted on the basis of the difference in duty. The cost for the low-temperature (LT) heat recovery was evaluated as one common train separate from the equipment associated with each gasifier train.

1.5.2 Acid Gas Removal

The AGR process for this H₂ production plant is a proprietary amine system. The cost basis used in the estimate is an estimate developed by the Parsons process group. The reference price was developed for another application. For this application, the cost was adjusted for the required capacity and inclusion of the H₂S furnace.

1.5.3 Sulfur Recovery and Tail Gas Cleanup

A sulfuric acid plant was specified to handle the gas from the AGR process. For this application, the cost is based on a budgetary quote provided by Monsanto. This furnished price was prepared

for a similar IGCC application and adjusted for this evaluation. The plant cost was adjusted for escalation and the change in plant capacity.

1.5.4 Hydrogen Purification

A PSA system was specified for the hydrogen purification process. The cost basis used in the estimate is based on a PSA system estimate developed by the Parsons process group. The reference price was developed for another application. For this application, the cost was adjusted for the significantly larger volumetric capacity (for both the Pittsburgh and Wyoak coals).

1.5.5 Shift Reactors

The shift reactor cost portion of the gas cleanup stream was based on cost information developed by the Parsons process group. The shift reactor portion that was part of another evaluation was utilized for this evaluation. In application for both coals, the cost was adjusted for somewhat smaller capacity of the reactors.

1.5.6 Candle Filters

The candle filters in the gas cleanup train were based on the cost of similar filters from other IGCC applications. The filter costs were originally based on pricing provided by Westinghouse and applied to the IGCC system requirements. These adjustments consisted of selecting the correct number of filter vessels to match the volumetric flow and candle type to match the temperature environment.

1.5.7 Air Separation Unit

The cost of the ASU portion of the gasification system was based on an in-house ASU cost model. This cost model was based on data provided by Air Products. The cost portion of the model was subsequently adjusted to reflect Parsons' experience with competitively furnished costs. The costs in this evaluation were adjusted for parameters such as capacity per day, purity, inlet pressure, and discharge pressure.

1.5.8 Balance of Plant

The costing of the balance of plant that constitutes the complete H₂ production IGCC was based on an in-house IGCC model that has been used to develop the capital costs and economic results for many IGCC applications. Each account within the model is adjusted to reflect the major cost parameter(s) for that component. Costs are adjusted on the basis of heat and mass balance data, equipment list, and plant arrangement drawing data.