

# Advanced Hydrogen and CO<sub>2</sub> Capture Technology for Sour Syngas

Final Report on Activities through 31 May 10

submitted to Alberta Innovates (formerly Alberta Energy Research Institute, AERI)

This is the final report describing Air Products work in the development of a new technology for treating sour syngas.

## 1. Background

A key challenge for clean power or hydrogen projects via gasification is the need to reduce the overall cost, while achieving significant levels of  $CO_2$  capture. The current technology option for capturing  $CO_2$  from gasification processes would be to selectively separate  $H_2S$  and  $CO_2$  from the  $H_2$ , usually by passing the gas into a physical solvent absorption process (acid gas removal – AGR) such as  $Selexol^{TM}$  or  $Rectisol^{\oplus}$ . These two processes are expensive and require significant utility consumption during operation, which only escalates with increasing levels of  $CO_2$  capture. Importantly, Air Products (AP) has developed an alternative  $CO_2$  capture option that can achieve a higher level of  $CO_2$  capture than the conventional technologies at significantly lower capital and operating costs. Overall, the system is expected to reduce the cost of  $CO_2$  capture by over 25% compared to the conventional technologies.

Air Products developed this novel technology by leveraging years of experience in the design and operation of H<sub>2</sub> pressure swing adsorption (PSA) systems in AP's numerous steam methane reformers (SMRs). Commercial PSAs typically operate on clean syngas and thus need an upstream AGR unit to operate in a gasification process. AP recognized that a H<sub>2</sub> PSA technology adapted to handle sour feedgas (Sour PSA) would enable a new and enhanced improvement to a gasification system. By combining the Sour PSA with a low-BTU oxyfuel burner technology and specialized CO<sub>2</sub> purification / compression system, the new system creates two significant values: 1) it eliminates the expensive AGR system and 2) it achieves higher CO<sub>2</sub> capture levels.

A general schematic of the flowsheet is shown in Figure 1, with the Sour PSA followed by the sour oxy-combustion unit and finally the  $CO_2$  purification / compression system. The Sour PSA is a multi-bed system capable of handling sour syngas ( $H_2$  / CO) containing  $CO_2$ ,  $H_2O$ ,  $H_2S$ , carbonyl sulfide (COS), carbon disulfide ( $CS_2$ ),  $CH_4$ , as well as other minor impurities. The  $H_2$  product purity is determined by the end use - high purity (99.99+%) for industrial refinery **Air Products Confidential** 

/ petrochemical use or lower purity for use as a gas turbine fuel. Essentially all the  $CO_2$  from the gasification system can be captured by combusting the PSA offgas using oxygen. The heat generated from the combustion system can be used for preheating streams to a turbine in a power system, steam generation, additional reforming in a hydrogen system, or any other ancillary use of high quality heat. The sour oxyfuel combustion is accomplished by combusting the waste gas with an excess of pure  $O_2$ , in which case the combustion products will be  $H_2O$ ,  $CO_2$ ,  $SO_2$ ,  $SO_3$  and excess  $O_2$ . The oxyfuel combustion may take place either in a once-through manner or with cooled flue gas recycle to moderate the combustion temperature.

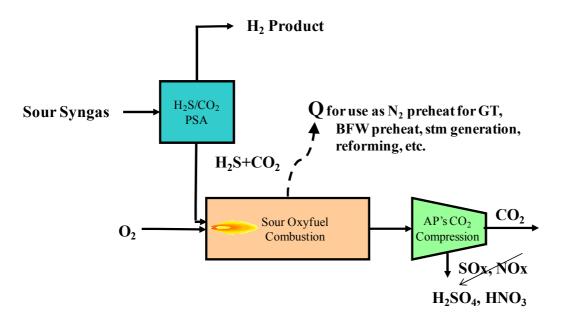


Figure 1: H<sub>2</sub> PSA offgas oxyfuel combustion for 100% CO<sub>2</sub> capture

The  $CO_2$  product gas may comprise a number of contaminants. For example, the gasification of petroleum coke (petcoke) or coal produces  $H_2S$  which, when combusted, produces  $SO_2$  and  $SO_3$  (or "SOx"). Excess  $O_2$  in the combustion step could result in  $O_2$  as a contaminant. The  $SO_2$  and excess  $O_2$  may be removed from the  $CO_2$  by processes applied during the compression sequence.  $SO_2$  is removed as  $H_2SO_4$ , and NO and  $NO_2$  are removed as  $HNO_3$  in that system. The  $SO_x$ -free,  $NO_x$ -lean  $CO_2$  gas may then be compressed to pipeline pressures and either stored in geological formations or used in enhanced oil recovery (EOR). The specialized  $CO_2$  purification / compression system, which includes  $SO_2$ ,  $NO_x$ , and inert removal systems, was originally developed by Air Products for oxyfuel  $CO_2$  capture for pulverized coal combustion power boilers but is well suited for the current application.

# 2. Description of Air Products Advanced CO<sub>2</sub> Capture (H<sub>2</sub>S / CO<sub>2</sub> Removal) Technology for Gasification

The process developed by AP combines the use of three novel elements which can be employed within the traditional gasification / power island flow sheet to reduce the costs of carbon capture. The three novel parts of the process are as follows:

- Sour Pressure Swing Adsorption (Sour PSA)
- Oxy-Sour Low Pressure Combustor with heat recovery
- SO<sub>x</sub> and NO<sub>x</sub> Reactor during CO<sub>2</sub> Compression

The Sour PSA is based on a traditional Hydrogen PSA for separation, which is a mature technology. AP has developed a novel material and cycle so the PSA can handle high concentrations of  $H_2S$  and COS in sour syngas from solid fuel or heavy resid gasification. Thus a hydrogen product is obtained and the tailgas contains the  $H_2S$  species. The sour tailgas is then combusted in excess oxygen in a novel combustor; which is operating at just above atmospheric pressure. The combustor fully converts all the sulfur species into sulfur oxides. Some nitrogen oxides ( $NO_X$ ) will be formed during the combustion process at conditions which promote the generation of the quantities required in the reactors downstream.

The tailgas combustor also represents an opportunity for heat integration / recovery which could be used for either steam generation (e.g., export steam or electrical power generation in a steam turbine) or as a heat source (e.g., preheating the H<sub>2</sub> or H<sub>2</sub>+N<sub>2</sub> fuel to the gas turbine) within the overall flow sheet. The combustion products, primarily CO<sub>2</sub> and H<sub>2</sub>O, will contain SO<sub>x</sub> and NO<sub>x</sub>. As CO<sub>2</sub> capture is part of the overall process, the combustion gases will need to be compressed and purified. Upon compression of the crude CO<sub>2</sub> stream, the increase in pressure and contact with water promotes a number of chemical reactions which convert all sulfur compounds to sulfuric acid and nitrogen oxides to nitric acid. The following figure outlines the pertinent equations and reaction characteristics of the conversion:

```
NO + \frac{1}{2}O_2
                                                         (1) Slow
                            NO_2
                                                          (2) Fast
2 NO<sub>2</sub>
                             N_2O_4
                            HNO_2 + HNO_3
2 \text{ NO}_2 + \text{H}_2\text{O} =
                                                    (3) Slow
3 HNO<sub>2</sub>
                             HNO_3 + 2 NO + H_2O
                                                         (4) Fast
NO_2 + SO_2
                             NO + SO_3
                                                          (5) Fast
                   =
SO_3 + H_2O
                   =
                             H<sub>2</sub>SO<sub>4</sub>
                                                          (6) Fast
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Figure 2. NO<sub>x</sub>/SO<sub>x</sub> reactions in the CO<sub>2</sub> compression system

The first zone for the reactions to occur in the oxyfuel purification process is after compression to 15 bar in the compression train. It is expected that the rate of Equation 1 will have increased sufficiently for it to require only a few seconds to reach equilibrium and convert most of the NO to  $NO_2$ , especially since there is sufficient  $O_2$  in the raw  $CO_2$  stream, due to the excess oxygen required for combustion. The second reaction of significance at this

<sup>&</sup>lt;sup>1</sup>Only feasible at elevated pressure

<sup>&</sup>lt;sup>2</sup>Rate increases with Pressure to the 3<sup>rd</sup> power

<sup>&</sup>lt;sup>3</sup>No Nitric Acid is formed until all the SO<sub>2</sub> is converted

<sup>&</sup>lt;sup>4</sup>Pressure, reactor design and residence times, are important.

point is the reaction of  $NO_2$  with  $SO_2$  to form sulfuric acid, commonly referred to as the lead chamber process for the manufacture of sulfuric acid. This reaction is known to be fast and so is considered to be equilibrium limited. Once all of the  $SO_2$  has been removed,  $NO_2$  will be converted to nitric acid by the well understood nitric acid process. These reactions give a path-way for  $SO_2$  to be removed as  $H_2SO_4$  and  $NO_3$  and  $NO_2$  to be removed as  $H_2SO_4$  and  $NO_3$  reactions.

The AP technology can be integrated into a gasification flow sheet with  $CO_2$  capture and can be evaluated as a replacement for the AGR in conjunction with other process integrations and improvements. Figure 3 shows the block diagram of the overall gasification process including the conventional technology as well as the AP process with  $CO_2$  capture. Two product types (power and hydrogen) can be used for base cases; 1. an IGCC with  $CO_2$  capture and 2. Gasification for  $H_2$  with  $CO_2$  capture. In particular, the base cases can be developed with petroleum coke as the feedstock and using conventional technologies for the AGR (e.g. Selexol<sup>TM</sup>). A detailed technical and economic comparison of the AP technology with the conventional technology is included in Section 4 of this report.

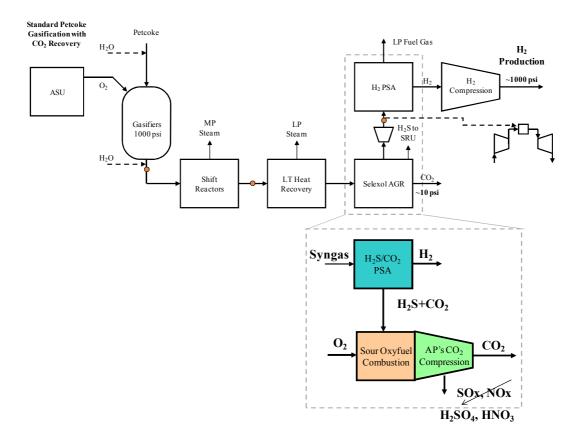


Figure 3: Block flow diagram for gasification for power or hydrogen with CO2 capture

# 3. Summary of Phase 1 Activities and Update on Progress

The Phase 1 activities are listed below with a high level status update. Subsequent sections of this report detail the current progress for each activity.

### Advanced Hydrogen and CO<sub>2</sub> Capture Technology for Sour Syngas

Phase 1: Feasibility Study					
Activities	Task Time (months)	Personnel (months)	Overall budget (\$kCAD)	Deliverables	Status:
Technical and economic feasibility study of conceptual commercial plant	3	6 (75% third party A&E)	170	Technical and economic feasibility study of conceptual commercial plant	Completed
Participate in experimental program at EERC.  Conduct additional validation tests for differing feedstocks (petcoke) than existing testing	3	3 & \$300k for EERC	440	Mobile PSA unit performance on sour syngas derived from petroleum coke	Completed
3. Pre-FEED design of prototype. Risk analysis and mitigation	12	12	300	Pre-FEED design of prototype. Risk analysis and mitigation plan	Initial concept sized. Technical risk assessment completed.
4. Select candidate sites in Alberta. Identify and validate options	6	2	55	List of candidate sites and an assessment of the site characteristics	Redirected to Activity 2/3
5. Identify and qualify potential first adopters	6	2	35	Prioritized list of first adopters	Redirected to Activity 2/3
Develop MOU with first     adopter committed to build     demonstration plant	6	3	35	MOU with first adopter	Redirected to Activity 2/3
7. Project Management	18	1	40	Status reports	Final report complete June 2010

Total \$1075 kCAD = (\$1,075,000 CAD)

# 4. Update on Progress for Phase 1 Activities

#### Activity 1: Technical and economic feasibility study of conceptual commercial plant

AP would work in conjunction with a third party A&E (proposed by AP and approved by AERI) to assess the technical and economic feasibility of a conceptual commercial plant. AP will provide sufficient technical data for proper assessment of the conceptual commercial plant. The conceptual commercial plant will be defined jointly by AP and AERI to address the Alberta market.

#### Update Activity 1: Scope of Work: Feasibility study of conceptual commercial plant

As part of activity 1 within the AERI / AP project, a technical and economic feasibility study of the conceptual commercial plant is required. AP worked in conjunction with Jacobs Consultancy to assess the technical and economic feasibility of a conceptual commercial plant. AP provided sufficient technical data for proper assessment of the conceptual plant. A kick-off meeting was held on 10 Dec 2008. The HAZID and flowsheet evaluation meeting were completed by the end of February. The final report was completed by the end of April and has been fully reviewed by Air Products.

Jacobs Consultancy used its knowledge in the fields of gasification, IGCC, combustor design, reactor design, product separation and heat integration to complete its work. The process optimization and integration is seen as an important step in the development of this technology. Jacobs' project scope and deliverables to Air Products are detailed below.

#### Project scope for technical and economic feasibility study of conceptual commercial plant

Initial process flow sheet:

- a. Identify and develop potential process flow schemes utilizing the AP advanced technology. This should include an evaluation of the process and heat integration opportunities across the whole plant enabled by the new technology.
- b. Generate the deliverables listed in section 4.0 for the novel process flow schemes identified. To ensure a meaningful cost comparison with the state-of-the-art, there should be two base cases developed with petroleum coke as the feedstock: 1. an IGCC with CO<sub>2</sub> capture (nominal 450 MWe) and 2. Gasification for H<sub>2</sub> with CO<sub>2</sub> capture (nominal 300 mmscfd H2). The advanced technology options and integration concepts identified will then be evaluated compared to the base cases.
- c. Identify the impact and uncertainty of key issues associated with the advanced technology (such as reaction chemistry / metallurgy etc). Any fatal flaws should be identified. Technical challenges should be identified along with recommendations on how to resolve them. Disposal/sale of sulfuric acid and nitric acid by-products should be addressed as well as other sulfur management options.
- d. Rank process flow sheet options and identify a preferred process configuration and level of integration.

e. Provide feedback on key process data required for detailed design, in order to influence the development program.

The following deliverables were completed by Jacobs Consultancy and are contained in Appendix A.

Phase 1 - Technical and economic feasibility study of conceptual commercial plant

- Basis of Design
- Process & Heat Integration Study
- Block Flow Diagrams
- Heat and Mass Balances
- Hazard identification (HAZID)
- Emissions and Flows at Battery Limits
- Utility Estimate / Plant Efficiency Evaluation
- Preliminary CAPEX Estimates (±50% accuracy)
- OPEX Estimates (±50% accuracy)
- Final Report

For this study Jacobs Consultancy evaluated four cases:

- Base Case with 4,473 STPD petcoke feed producing 273 MMSCFD H2 [Conventional Technology for Hydrogen Production]
- Base Case with 4,473 STPD petcoke feed producing 453 MW net power [Conventional Technology for Power Generation]
- Sour PSA Case with 4,473 STPD petcoke feed producing 268 MMSCFD H2 [Air Products Sour PSA Novel Technology for Hydrogen Production]
  - Oxy-combustor superheats LP and HP steam, excess heat used to generate and superheat additional HP steam. Steam used to generate power in steam turbine block.
  - Condensing economizer on oxy-combustor flue gas
  - o Dilute acid products neutralized or landfilled
- Sour PSA Case with 4,473 STPD petcoke feed producing 473 MW net power [Air Products Sour PSA Novel Technology for Power Production]
  - Oxy-combustor superheats LP and HP steam, excess heat used to generate and superheat additional HP steam. Steam used to generate power in steam turbine block.
  - o Condensing economizer on oxy-combustor flue gas
  - o Dilute acid products neutralized or landfilled

Block flow diagrams for the four cases are shown in Figures 4, 5, 6, and 7. More detailed diagrams are attached in Appendix A.

Given the time schedule, full optimization was not possible. In addition, not all fruitful process options could be evaluated. Therefore, the four cases were selected to help in the evaluation and to aid in identification of key items that warrant further work based on their impact to the project economics. Air Products valued the work by Jacobs Consultancy as it has helped to focus the next steps for successful development of the technology. In particular, the end use of the byproducts from the process is key to maximizing economic value.

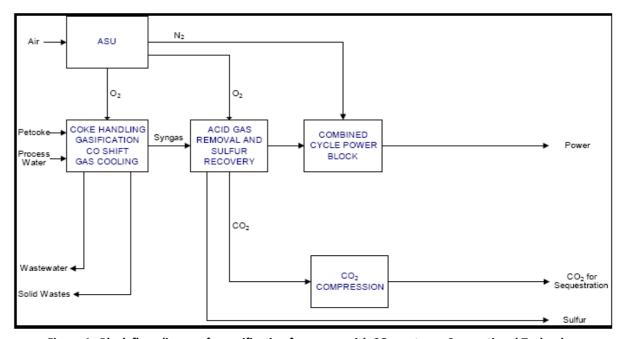


Figure 4: Block flow diagram for gasification for power with CO<sub>2</sub> capture: Conventional Technology

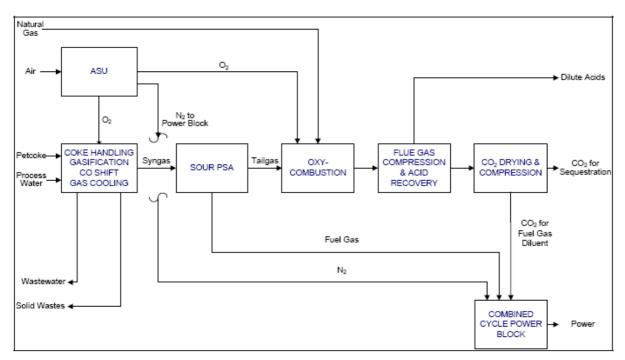


Figure 5: Block flow diagram for gasification for power with CO<sub>2</sub> capture: AP Technology

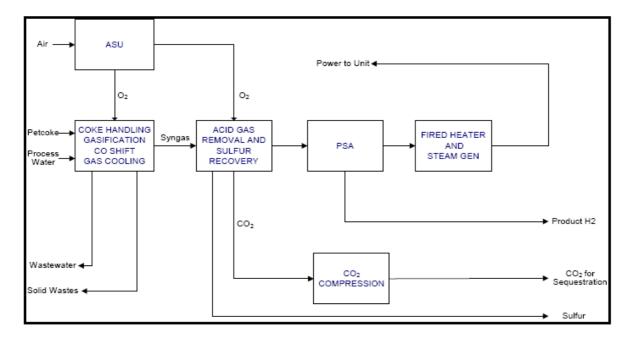


Figure 6: Block flow diagram for gasification for hydrogen with CO<sub>2</sub> capture: Conventional Technology

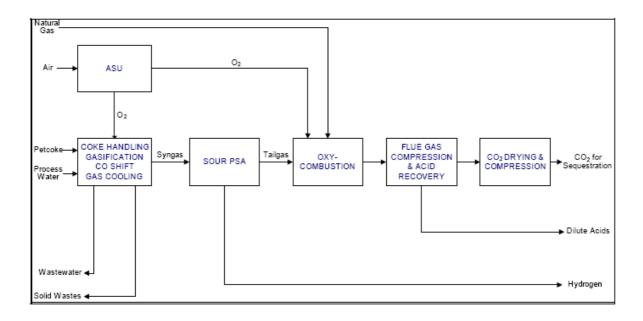


Figure 7: Block flow diagram for gasification for hydrogen with CO<sub>2</sub> capture: AP Technology

To aid Jacobs Consultancy's evaluation of the technology options, a series of sour PSA simulations were conducted by Air Products for petcoke gasification using APCI's novel technology. Several iterations were completed in order to understand the sensitivity of the PSA process cycle on the overall flow sheet.

#### **PSA Simulations**

Air Products has developed a dynamic adsorption process simulation tool called SIMPAC to help design and troubleshoot our numerous  $H_2$  pressure swing adsorption plants. The model solves the unsteady-state heat, mass, and momentum equations that describe the progression of concentration and thermal fronts along a fixed bed adsorber. The simulator can be applied to all of the common steps of a PSA – feed, pressure equalization, purge, depressurization and repressurization. It can also simulate consecutive series of these steps (cycles) until the system achieves 'cyclic steady state', a point where the dynamic concentration and temperature profiles for each step are identical to the profiles calculated for the previous cycle. This is the solution that describes performance of an industrial unit. Overall process performance can then be determined by evaluating the cumulative inlet and outlet gas flows and compositions, which then lead to tangible parameters such as  $H_2$  recovery ( $H_2$  in product divided by  $H_2$  in feed), bed loading (Ibmoles of feed processed per hr per ft<sup>3</sup> of bed), and carbon rejection (moles of CO, CO<sub>2</sub> and CH<sub>4</sub> rejected to low pressure waste stream divided by the amount in the feed gas).

Simulations were conducted for three scenarios studied by Jacobs Consultants: Case 1: H<sub>2</sub> production via sour PSA, Case 2: Power production via sour PSA, and Case 3: H<sub>2</sub> production via post Rectisol® PSA. The PSA feed gas composition, pressure and temperature for each case were obtained from Jacobs and are listed in Table 1.

Table 1. Feed Gas for PSA Processes.

	H <sub>2</sub> : Case 1, 2 stage WGS	Power: Case 2, 1 stage WGS	Power: Case 2, 2 stage WGS	Post Rectisol®: Case 3, 2 stage WGS
H <sub>2</sub>	54.154	52.5336	53.599	95.412
N <sub>2</sub>	0.318	0.772	0.755	0.56
СО	1.275	3.572	1.245	2.247
CO <sub>2</sub>	42.685	40.929	42.259	1.509
CH4	0.046	0.046	0.045	0.079
Ar	0.107	0.679	0.664	0.193
H <sub>2</sub> S	1.247	1.259	1.234	0
cos	0.002	0.0054	0.0023	0
H₂O	0.166	0.204	0.197	0
P (atm)	64.15	64.15	64.15	64.15
T (F)	112	119	118	111

PSA simulations were conducted to provide relevant process data for Jacob's ASPEN process simulations (*i.e.*, to determine the split of each feed component into a high pressure product stream and a low pressure waste stream). The sour PSA units were targeted for at least 90% carbon rejection. The H<sub>2</sub> product specification was 1 ppm CO + CO<sub>2</sub>. A standard 10-bed H<sub>2</sub> PSA cycle was used in all of the simulations.

#### Case 1: H<sub>2</sub> production via sour PSA

In this case the sour PSA is designed to remove essentially all of the syngas impurities to produce a high purity  $H_2$  product gas. A large part of the optimization was associated with proper specification of the adsorbent layers. Once the bed loading was fixed, a series of simulations were conducted at different purge flow rates to determine the optimum operating conditions that maximized  $H_2$  recovery.

#### Case 2: Power production via sour PSA

In this case the sour PSA product gas is considered decarbonized fuel, and is combusted in a gas turbine to produce power. The PSA separation requirement is dramatically reduced – key performance factors are to remove enough  $CO_2$  from the product gas to achieve 90% carbon rejection and to limit the  $H_2S$  level in the product to < 3 ppm (to satisfy assumed  $SO_x$  emissions levels in the turbine flue gas). A single layer of adsorbent is capable of achieving these targets. A series of simulations were conducted at different purge flow rates to determine the optimum operating conditions that maximized  $H_2$  recovery.

The results of initial PSA simulations for this case indicated that relatively high carbon rejection levels could be achieved, > 95%. We therefore focused on gasifier schemes with a single stage of WGS reaction rather than the more typical multistage WGS assembly – there was no justification to shift additional CO in the second stage since the incremental carbon it represented was tolerable in the product gas and the cost savings were appreciable.

#### Case 3: H<sub>2</sub> production via post Rectisol® PSA

In the final case, the PSA treats relatively pure feed gas from a Rectisol® unit to produce high purity  $H_2$ . There is no significant  $H_2$ S or COS in the feed, so this looks more like a conventional  $H_2$ PSA rather than a sour PSA. Simulations were also conducted at different purge flow rates to determine the optimum operating conditions that maximize  $H_2$  recovery.

Once all of the above simulations were completed, the PSA process could be scaled against the required feed flows from the power process simulations. Occasionally industrial flows are too large to handle in a single assembly (or train) of PSA vessels (due to limitations in vessel diameter). Multiple PSA trains are then required as was the case for all three PSA applications.

Capital costs for the PSA unit were evaluated once the vessel size and number of required trains was determined. An in-house program was used to estimate costs of adsorbent, vessels, valves, valve skid, and control equipment. An installed capital cost was determined by applying an installation factor typical for PSA systems. Costs were evaluated for the high pressure feed case only.

A summary of the performance parameters and relative costs is listed in Table 2. Hydrogen recovery is in the normal 85-90% range for the H<sub>2</sub> product cases, but it is much higher for the power case where some of the impurities can slip to the product. Carbon rejection is 92% in the power case, and essentially 100% in the sour PSA for H<sub>2</sub> case. The relative feed loading results show that sour PSA units have lower loading than the post Rectisol® PSA. This is due to the much higher impurity level of the sour feed gases. Operation at lower feed gas pressure yields some improvement in H<sub>2</sub> recovery at the expense of substantial reduction of bed loading (i.e., bigger vessels). The relative capital costs show that sour PSA options are 2-3 times more expensive than the post Rectisol®PSA. Of course, the sour PSA process eliminates the need for the Rectisol® unit with its associated capital cost and energy intensity, so the overall power or H<sub>2</sub> production process costs are offset.

Table 2. Summary of PSA Simulation Results.

	Feed Pressure (atm)	H₂ Recovery %	H <sub>2</sub> Product Purity %	Carbon Rejection %	Relative Feed Loading	Relative Capital Cost
Sour PSA for H <sub>2</sub>	64.2	85.6	99.96	100.0	0.56	3.15
Sour PSA for Power	64.2	92.3	91.32	92.6	0.78	2.34
Sour PSA for Power	33.0	95.6	91.20	92.1	0.47	
Post Rectisol PSA for H <sub>2</sub>	64.2	87.2	99.90	100.0	1.00	1.00
Post Rectisol PSA for H <sub>2</sub>	33.0	87.9	99.89	100.0	0.60	

These results from the PSA simulations were supplied to Jacobs for their evaluation. In addition, both capital and operating costs for the required  $O_2$  supply (cryogenic air separation units (ASUs)) were provided.

Jacobs evaluated the four cases as described previously:

- Base Case with 4,473 STPD petcoke feed producing 273 MMSCFD H<sub>2</sub> [Conventional Technology for Hydrogen Production]
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The overall capital and operating & maintenance costs were calculated and are shown in Tables 3 & 4 (excerpts from the Jacobs study - Appendix A). These results are useful in comparing technologies and identifying where efforts should be made to reduce costs. No project net present value calculations were done within the Jacobs study as values for CO<sub>2</sub> capture amounts or excess power sales or hydrogen sales were not within their scope. A brief analysis will be described later, which will link to the current technology development plan.

Table 3. Capital Costs from Jacobs Study (Appendix A).

Case	Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
	\$ million	\$ million	\$ million	\$ million
Air Separation Unit	316.7	307.1	343.0	330.9
Petcoke Receiving, Storage & Handling	19.0	19.0	19.1	19.1
Gasification Including Feed Preparation	286.1	237.0	286.1	237.0
Gas Cooling and Shift Conversion	273.0	275.0	273.0	233.7
Acid Gas Removal*	286.3	288.4		
Sulfur Recovery	122.7	122.7		
Hydrogen Purification	49.0			
Sour PSA			154.4	115.0
Sour Gas Oxy-Combustion			108.3	98.4
Flue Gas Compression & Acid Recovery			146.6	146.6
CO <sub>2</sub> Drying & Compression	60.6	58.4	15.5	14.8
Power Block	45.3	418.6	61.3	453.1
Utilities & Support Facilities	366.8	431.6	349.4	409.9
Field Costs	1,825.5	2,157.8	1,756.5	2,058.5
Home Office Costs	275.1	323.7	263.5	308.8
Construction Management Costs	55.0	64.7	52.7	61.8
Overall Project Management Contractor Costs	108.2	127.3	103.6	121.4
Total before Contingency	2,263.8	2,673.5	2,176.2	2,550.4
Contingency	454.5	534.7	435.2	510.1
Project Total Installed Cost	2,718	3,208	2,612	3,061

Note: Air Products also has experience with Rectisol® units, and there were slight differences between the estimated capital costs for the Rectisol® system. For consistency, Jacobs Consultancy's estimated capital cost was used; differences may occur with regard to efficiency of refrigeration and alternate regeneration methods, among other reasons.

Table 4. Operating & Maintenance Costs from Jacobs Study (Appendix A).

Case	Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
	\$ million/yr	\$ million/yr	\$ million/yr	\$ million/yr
Net Imported Power	60		38	
Natural Gas			14	30
Sulfur Disposal	1	1		
Acid Neutralization Costs:				
Limestone			30	30
Gypsum Shipping			6	6
Other O&M Costs	136	160	131	153
Annual O&M Costs	197	162	218	218

Note: Does not include the extra 20  $MW_e$  produced by the Sour PSA Power case. Assumes maximum trim fuel firing rate and the use of natural gas rather than a lower cost fuel.

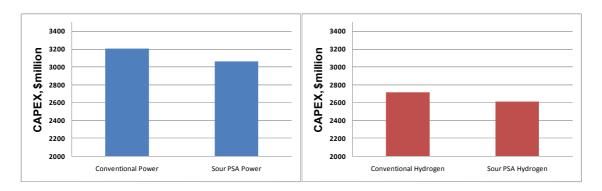


Figure 8: Capital Costs from Jacobs Study (Appendix A).

Both Table 3 and Figure 8 show that the AP technology cases had lower Capex than the conventional technologies (savings of ~\$147 million for power and ~\$106 million for hydrogen). However, as shown in Table 4 and Figure 9, the operating & maintenance costs were higher for the AP technology (penalty of ~\$56 million for power and ~\$21 million for hydrogen). Clearly, the operating & maintenance costs must be reduced. After discussion with Jacobs and further analysis, Air Products has identified two categories; scope impacts and future improvements. The scope impacts were areas that were not covered by the Jacobs study, but impacted the operating & maintenance costs. For example, the Air Products' Power case produce 20 MWe more power than the Conventional Technology Power case. That extra power was not included in any analysis. At nominal power sales rates, the extra power would be worth ~\$14 million per annum. In addition, the operating expenses of the Sour PSA system are higher than the conventional system due to the costs of neutralization and disposal of the sulfuric acid, which total approximately \$36 million per annum. Alternative uses for the sulfuric acid were investigated, but given the study schedule, the use of neutralization and disposal of the sulfuric acid was the expedient choice. However, use of the byproduct acid for other industries would dramatically lower the effect on the operating & maintenance costs. Next, the trim fuel flowrate necessary for the oxy combustion system was very conservative. Based on experiments performed at Air Products on oxy-combustion of low BTU fuel gas, it is now believed that less trim fuel is needed. Also, natural gas was used as the trim fuel to simplify the study, but it may be replaced by lower cost fuels (e.g., sour RFG or sour syngas). These fuel changes can directly affect the operating & maintenance costs by up to \$15 million per annum. Finally, the effective higher capture rates with the new technology were not valued in any way in this study as they were outside of the Jacobs scope and since the higher capture rate has a concomitant higher compression power, an added artificial penalty resulted. Air Products also has experience with Rectisol® units, and there were slight differences between the estimated capital and operating costs for the Rectisol® system. Therefore, the updated operating & maintenance costs (including the above changes) are shown in Figure 9 as the third columns. Now the operating & maintenance costs are nominally lower for the AP technology (savings of ~\$2 million for power and ~\$24 million for hydrogen).

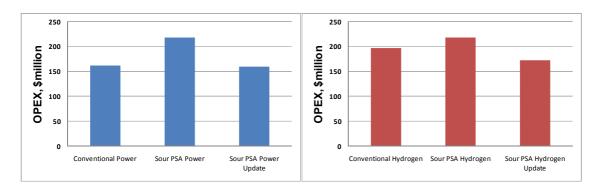


Figure 9: Updated Operating & Maintenance Costs.

Both Jacobs and Air Products identified many ways to improve the AP technology. One area is to continue to reduce capital costs, especially for the Sour PSA and the CO<sub>2</sub> compression system. In addition, the high sulfur content in the petcoke produced more acid than with lower sulfur solid fuels, so other options should be considered. The heat from combustion of the sour offgas could also preheat the gas turbine fuel for the power cases, not just raising/superheating steam. Also, the CO<sub>2</sub> compression system costs were higher for the sour PSA because the compression system being used was optimized for oxycoal. AP needs to look at different configurations to get lower power consumption (*e.g.*, having one column and using four stages with intercooling for the compression). Further reductions in compression equipment costs are possible. Identification and development of options related to removal of the sulfur components in the Sour PSA tailgas could reduce the operating expenses and may reduce the capital costs. Some options include PSA advancements, such as two stage systems that would remove H<sub>2</sub>S as well as hydrogen, and compression and co-injection of H<sub>2</sub>S and CO<sub>2</sub> into sequestration wells.

A non-ranked listing of further options to consider is included below:

- Other uses for acids (fertilizer, ammonia, etc.)
- Use of ash from a nearby power plant for acid neutralization (conventional pulverized fuel power plant)
- Use of the low-grade heat generated in the oxy-combustor and gasification sections for acid concentration
- Two-stage PSA: first stage CO<sub>2</sub> rejection, second stage for H<sub>2</sub> purity
- Two-stage PSA: first stage H<sub>2</sub>S removal to Claus unit, second stage for H<sub>2</sub> purity
- Two-stage PSA: Within an upgrader, use the first PSA to achieve the power block feed composition (within the H<sub>2</sub>S limits), and the second PSA to get product H<sub>2</sub> purity
- Purge the PSA with CO<sub>2</sub> instead of H<sub>2</sub> for higher CO<sub>2</sub> purity

- Purge the PSA with N<sub>2</sub>
- Licensed ammonia scrubber technology to convert SO₂ to ammonium sulfate for fertilizer
- Licensed technology to treat the flue gas by converting  $SO_2$  to concentrated, high-purity sulfuric acid and in addition converting  $NO_x$  to  $N_2$
- Wet limestone scrubbing of oxy-combustor flue gas
- Increased sour PSA tailgas pressure to reduce compression costs; trade-off is lower recovery within the PSA and higher pressure oxyfuel combustion
- First stage of compression upstream of the oxyfuel combustion
- Mercury removal before the Sour PSA or membrane WESP (claims to remove Hg)
- Use of the oxyfuel combustor heat to superheat steam at various pressures rather than making only saturated steam

Air Products has prioritized the above technology options while considering their potential scope impact and congruence with the overall technology and commercialization strategy. Several of the options are at various stages of development.

# Activity 2: Participate in experimental program at EERC. Conduct additional validation tests for differing feedstocks than existing testing (Mobile PSA testing at EERC)

#### Goals

- 1. Evaluate performance of a Sour PSA/TSA utilizing syngas feed from a petcoke gasifier
- 2. Determine appropriate regeneration mode for adsorbents (PSA/TSA)
- Generate process data for petcoke-derived syngas that can be correlated for future scaleup

#### **Update Activity 2: Experimental Progress**

#### Sour Pressure Swing Adsorption (PSA) Process Development

The goal of this work is to develop a PSA process that can treat sour syngas from a coal or petcoke gasifier to produce an enriched hydrogen product and a sour  $CO_2$  byproduct. The enriched  $H_2$  product can contain some of the carbon species in the feed (e.g., CO,  $CH_4$ ), but the overall carbon rejection is targeted for 90% or better. It will be of sufficient quality to be combusted in a gas turbine for clean power generation. All sulfur species (and other trace syngas contaminants) are to be rejected to the  $CO_2$  byproduct stream. This stream will undergo further treatment to produce a purified and compressed  $CO_2$  stream for sequestration.

The steps in the sour PSA development activities have proceeded as follows:

- Assess the performance of high-temperature and conventional CO<sub>2</sub> sorbents in simulated synthesis gas (syngas)
- Evaluate the effect of H₂S on most promising adsorbents when operating in a fixed-bed under real syngas conditions
- Assess the performance of most promising adsorbents during long-term exposure to low levels of impurities (i.e., iron carbonyl, carbonyl sulfide, and hydrogen fluoride)

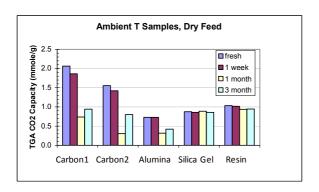
Throughout the above development activities AP has estimated the potential industrial PSA performance of the most promising adsorbents with a process simulator and validated the simulation parameters by comparing with real process data. Additionally, key adsorbent characteristics were evaluated throughout the campaigns by means of carefully controlled breakthrough experiments and adsorbent post-mortem analysis. The details and results of each of the activities are detailed below.

The first step in sour PSA development activities was to identify and demonstrate what types of adsorbents can be used for this application. Phase 1 of the development activities consisted of extended (six months) exposure testing of potential adsorbent materials to synthetic sour gas. Most of the adsorbents showed an increase in sulfur content, and subsequent decrease in surface area and CO<sub>2</sub> adsorption capacity with exposure. However, two adsorbent materials were identified which were stable in a blended sour syngas over the six month period.

Figure 10 below shows the exposure apparatus that was set-up at the Energy and Environmental Research Center (EERC) in Grand Forks, ND. Over a six month period five candidate adsorbents (two carbons, alumina, silica gel, and polymeric resin) were exposed to a blended sour gas at ambient temperature and 400 psig. The synthetic sour gas consisted of 1% H<sub>2</sub>S, 8% CO, 37% CO<sub>2</sub>, and balance H<sub>2</sub>. Throughout the exposure testing the samples were periodically analyzed for CO<sub>2</sub> capacity, surface area, and sulfur content. The results presented in Figure 11 show the silica gel and polymeric resin perform well when exposed to sour syngas and were selected as the most promising candidate for further analysis in fixed-bed testing with real syngas.



Figure 10. Ten-bed exposure unit at EERC.



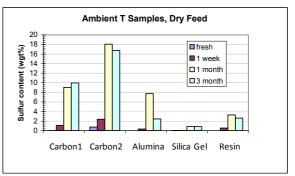


Figure 11. Results of adsorbent stability testing.

In the second phase of testing, a two-bed Sour PSA test unit was constructed and interfaced with a continuous fluidized bed gasifier (CFBR) at EERC. The EERC CFBR can process 4 lb/hr coal in  $O_2$  or air-blown mode. A schematic drawing and photo of the CFBR unit are illustrated in Figure 12 and 13. Reactants (steam,  $O_2$ ) and fluidization gases (recycled syngas) are introduced at the bottom of the reactor. A gas booster (not shown) is used to compress the recycle gas. The reactor consists of sections of 3 and 4 inch Sch80 316H pipe. It is externally heated with ceramic fiber heaters to minimize hot spots. The reactor can operate at up to 150 psig and 870°C. Solids are removed in a heated cyclone and the gases are passed to a sour shift unit for CO conversion to  $CO_2$  and  $CO_2$  and  $CO_3$  are removed in a series of quench tanks and knock-out pots that are all water-cooled. At this point the cooled syngas is fed to the gas booster for recycle. A portion of the compressed recycle gas (~600 psig) is sent to the sour PSA unit as feed gas. The gasifier can deliver 10-15 slpm feed gas in this manner.

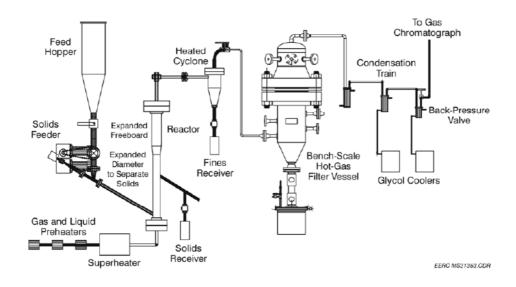


Figure 12. Schematic of EERC Continuous Fluidized Bed Gasifier.

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Figure 13. Photo of EERC CFBR.

The sour PSA unit is designed to test the performance of various adsorbent materials under PSA or TSA conditions with sour syngas from the gasifier. The PSA unit consists of two insulated and electrically heated columns, a set of air-actuated switching valves at the top and bottom of the column, feed and purge gas mass flow controllers, various process tanks (product, depressurization, and purge), effluent gas flow meters, and analytical detectors (micro GC and CO IR unit). A schematic and photograph of the unit is illustrated in Figures 14 and 15.

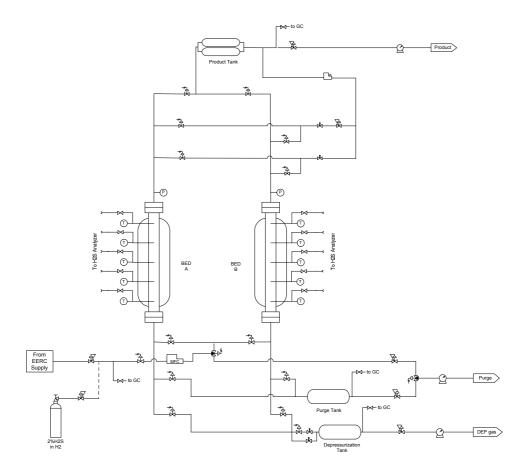


Figure 14. Schematic of Sour PSA Unit.



Figure 15. Photo of Sour PSA Unit.

The vessels can be operated as a pressure swing adsorption unit or a thermal swing adsorption unit (although the latter mode has not been implemented in this work). In PSA mode each bed sequentially progresses through the following process steps;

- 1) high pressure feed (normally 400 psig),
- 2) countercurrent depressurization (to ~1-10 psig),
- 3) countercurrent low pressure purge (1-5 psig) with product gas,
- 4) countercurrent repressurization with product gas.

Operation of the fixed-bed unit is conducted through a PLC system which automatically executes the proper valve and heater sequencing for the chosen cycle. The operator must set the time lengths of the various steps, the feed flow rate, the purge gas flow rate (via a manual purge valve), the repress rate (via a manual repress valve), and the depressurization gas flow rate (via a set of parallel manual depress valves). Gas pressure during each step is controlled by back pressure regulators. Gas flow rates and compositions can be determined for the feed, product,

purge effluent and depress effluent streams. This permits evaluation of overall and component mass balances and estimation of  $H_2$  recovery /  $H_2$ S rejection.

The major objectives of putting these two units together was to evaluate adsorbent stability to coal-derived syngas under PSA conditions, conduct H<sub>2</sub>S breakthrough tests under controlled adsorber conditions, and to obtain PSA performance data that can be used to validate our adsorption process simulation model. The feed to the CFBR gasifier was Powder River Basin (PRB) coal spiked with elemental sulfur to yield between 1-3% H<sub>2</sub>S in the gasifier effluent (coal analysis for typical PRB sample is listed in Table 5). The effluent from the gasifier was passed through a sour shift reactor and water-cooled quench tanks before being sent to the PSA at 400 psig and ambient temperature. During the first four week campaign of combined gasifier and PSA testing, a total of 1220 cycles were completed with the PRB coal syngas. Appendix B shows the results of a detailed analysis of the coal-derived syngas performed by an external analytical lab. They show the expected syngas components CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, and inerts, as well as H<sub>2</sub>S, COS, and low levels of mercaptans. More surprising was the appearance of ~600 ppm benzene, along with trace levels of toluene, ethylbenzene, xylenes, and naphthalene. Additionally, gas chromatography was used to routinely monitor the major components of the PSA feed gas during testing.

Table 5. Proximate analysis of typical PRB coal.

## Rochelle coal, Antelope mine

Proximate Analysis, wt%		Ash Compsition, % as oxides			
Moisture	23.4	Calcium, CaO	29.7		
Volatiles	33.8	Magnesium, MgO	10.1		
Fixed Carbon	37.3	Sodium, Na2O	1.43		
Ash	5.5	Silica, SiO2	22.5		
		Aluminum, Al2O3	13.8		
<b>Ultimate Analysis</b>	, wt%	Ferric, Fe2O3	8.4		
Carbon	51.7	Titanium, TiO2	1.2		
Hydrogen	6.2	Phosphoros, P2O5	1		
Nitrogen	0.9	Potassium, K2O	0.4		
Sulfur	0.2	Sulfur, SO3	11.4		
Oxygen	35.5				
Ash	5.5	HHV, Btu/lb	8770		

Following the first campaign, the columns were removed, capped, and sent to APCI labs for post mortem analysis. A controlled suction device was used to remove adsorbent from the feed end of each bed. An illustration of portions of the solid samples taken from columns A and B is shown in Figure 16. There is an obvious orangish-yellow color for the samples near the feed end of the bed. A hydrocarbon odor was noted when sampling the columns which is most likely attributed to the heavier aromatic components observed in the syngas feed analysis.

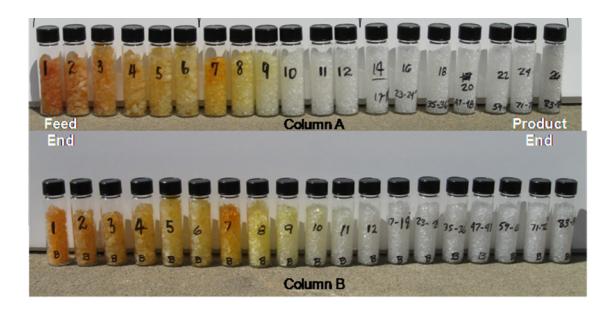


Figure 16. Spent Adsorbent Samples from EERC Columns A & B (coal-derived syngas).

Select samples from Bed A were submitted for XRF analysis. The results, illustrated in Figure 17, show increased levels of sulfur and chlorine in the 1<sup>st</sup> layer of adsorbent. Chlorine does not appear to make it to the 2<sup>nd</sup> layer of adsorbent, consistent with decreasing concentration profile in the 1<sup>st</sup> layer. Sulfur, however, is present at higher levels than the fresh material for the first few samples of the 2<sup>nd</sup> layer, indicating that it has broken through the first layer.

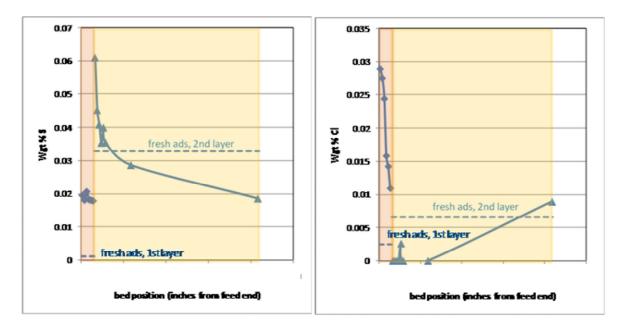


Figure 17. Sulfur and Chlorine Loading of Used Adsorbent Bed, XRF analysis.

An analysis of the adsorption capacity of select samples was also conducted by measuring both the surface area (via BET approach) and the  $CO_2$  adsorption capacity (TGA experiments,  $CO_2$  uptake at ~1 atm pressure and  $30^{\circ}$ C). The results indicate that the accumulation of sulfur and chlorine components on the adsorbent does not negatively impact its adsorption capability – in fact in most cases there appears to be an overall increase in  $CO_2$  capacity. Results are plotted in Figure 18.

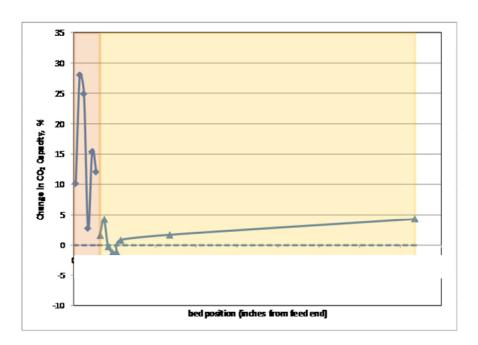


Figure 18. Impact of Sour Syngas Exposure on CO<sub>2</sub> Capacity.

During the first campaign of testing it appeared that the  $H_2S$  capacity of the adsorbent decreased by approximately 20% between cycles 0 and 1220. Because  $H_2S$  breakthrough experiments were only conducted at the start and end of the campaign, it was unknown whether the decrease occurred rapidly followed by stabilization or continually declined over the testing period. To better understand these phenomena, a second campaign was conducted at EERC using the same gasifier and PSA set up as before, but with a new protocol to run intermittent  $H_2S$  breakthrough experiments during the campaign to monitor the  $H_2S$  capacity over time.

Once the PSA was loaded with fresh adsorbent (same layering as the first run) and sent back to EERC, the second coal campaign resulted in approximately 1500 cycles being completed on the PSA. The results of the  $H_2S$  breakthroughs for the first and second campaigns are shown in Figure 19a. The red data in the figure are from the first campaign, they show a drop of about 20% relative to the fresh adsorbent. The blue data are from the second campaign. The second campaign results suggest that there is an accumulation of sulfur- and chlorine-containing components on the feed-end of the adsorbent bed. Presumably this is what leads to the coloration of these

samples. This accumulation does not appear to significantly impact the  $CO_2$  adsorption properties of the material. It is likely that these components are retained on the surface of the adsorbent rather than throughout the bulk of the silica. The new results suggest that the capacities decrease during the first 700 cycles, and then stabilize with further cycles.

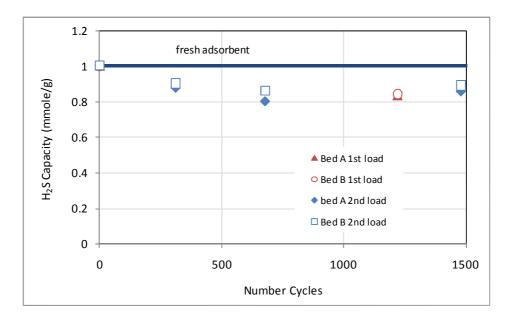


Figure 19a: H<sub>2</sub>S Capacity from Breakthrough Tests (Gasifier Syngas).

The columns used during the second coal campaign were thermally regenerated at 120°C (column A) and 200°C (column B), removed from the unit and shipped to APCI for unloading. We removed the spent adsorbent with a vacuum tube assembly that permitted sampling every inch of the column. We noticed that these samples were not as yellow as the previous samples from the 1<sup>st</sup> campaign. They were more of a brown color, particularly the 200°C regenerated sample.

The properties of the spent samples from both coal campaigns were determined by TGA analysis and headspace gas chromatrography. TGA analysis was conducted by first heating the sample in 200C  $N_2$  for 30 min, cooling to 40C in  $N_2$ , switching to 30 min of 100%  $CO_2$  at 40C followed by 30 min in  $N_2$ . The mass change during the  $CO_2$  feed and the last  $N_2$  purge were recorded and compared to values obtained for fresh adsorbents. The relative change between spent and fresh samples is plotted in Figure 19b. The x axis indicates the position of the sample in the bed, where zero corresponds to the feed end. The results for the first bed loading show an increase in the first 10 inches of the bed, but the  $CO_2$  capacity of samples further down the column were similar to fresh material. The second load columns were thermally regenerated in  $N_2$  at the end of the cycling experiments, the first bed represented by the green data points was heated to 120C and the second bed represented by red symbols was heated to 200C. The data appear to be somewhat contradictory, as the non-regenerated samples (blue symbols)

indicate that the spent samples have higher capacity than the fresh samples. The regenerated samples suggest a loss of capacity by about 5-20%. More TGA experiments need to be run for the non-regenerated (blue symbol) and 120C treated (green symbol) data between 10 and 50 inches.

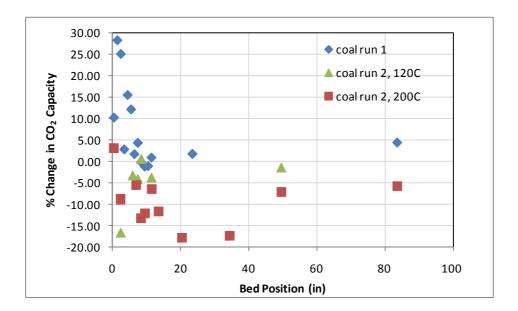


Figure 19b. Change in CO<sub>2</sub> capacity for spent adsorbent samples.

Headspace analysis of the spent samples was requested in order to get an idea of what was adsorbed on them. A typical GC analysis is plotted in Figure 19c which shows that many types of hydrocarbon species are present – too many to accurately quantify. We instead combined the species into groups of aromatics, indanes, tetrahydronaphthalenes (THN) and naphthalenes (Naph).

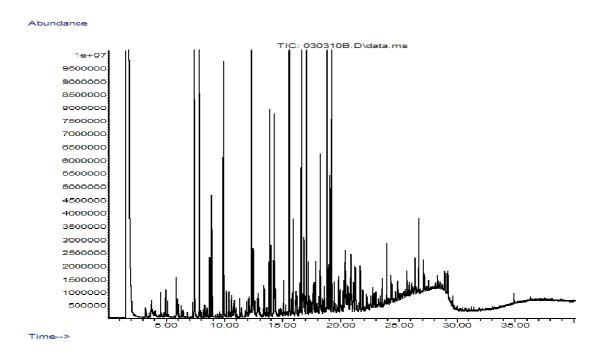


Figure 19c. Headspace GC chromatogram for a spent adsorbent sample.

Area counts observed for these groups as a function of the column position are illustrated in Figure 19d for the two regenerated column samples. Aromatics and indanes are the most plentiful species, and they are concentrated towards the feed end of the columns. Regeneration at 200C appears to have removed some of these hydrocarbons, especially with respect to the lower boiling aromatics and indanes. It is expected that the presence of these large aromatic species would negatively impact the adsorption of smaller species (e.g., H<sub>2</sub>S) via pore blocking or taking up of adsorption space. The data, however, are somewhat inconsistent on this point as the more loaded samples from the 120C regen test seem to show higher CO<sub>2</sub> capacity via the TGA testing. It seems reasonable, however, to at least in part associate the 20% decrease in H<sub>2</sub>S capacity observed with the breakthrough tests (Figure 19a) to the loading of the adsorbent with these large tar species.

It is important to remember that these results were obtained from the lignite campaigns with the CFB gasifier – tar production was severe under these conditions. A similar post mortem analysis will be conducted with the columns from the petcoke-based testing once it is complete.

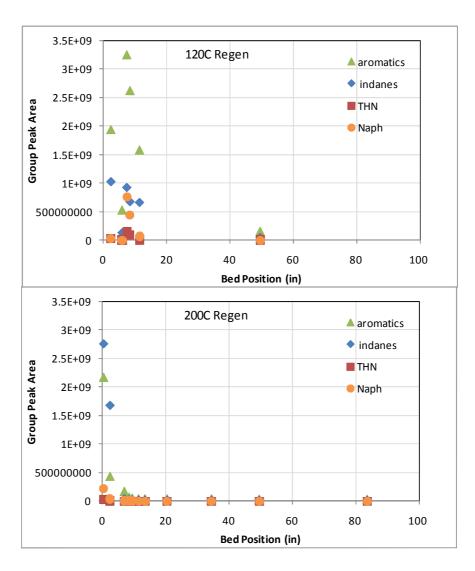


Figure 19d. Headspace analysis results for spent adsorbent samples.

The third phase of testing consisted of interfacing EERC's entrained flow gasifier (EFG) with the Sour PSA. For this campaign, both columns of the sour PSA were once again loaded with fresh silica gel. The EFG, pictured schematically in Figure 20, can process 8 to 10 lb/hr petcoke in  $O_2$  or air-blown mode at a higher pressure (300 psig) than the CFBR. Higher temperatures of up to 1500C are attainable with external electrical heaters in the gasifier wall. Like the CFB unit, syngas from the EFG is shifted in a sour shift reactor and a portion is compressed and recycled to the gasifier. This recycle gas is used to purge various electrical throughways that penetrate the gasifier, as well as solids inlets. A portion of this recycle gas was taken as feed gas for the sour PSA unit.

Interfacing with the EFG is advantageous for this study as it can best accommodate a Canadian petcoke feedstock, allowing further study of the effects of various syngas compositions on the stability of the adsorbent. According to the petcoke provider, Suncor, the petcoke consists of a typical sponge coke, with low ash content (2 -3%), a HV

energy content of 13,500 BTU/lb and lots of vanadium and nickel. Suncor states a sulfur content of the petcoke of around 6%. The coke was delivered in 22 55-gallon drums in chunk form, and was ground at EERC to 200 mesh for use in the gasifier.



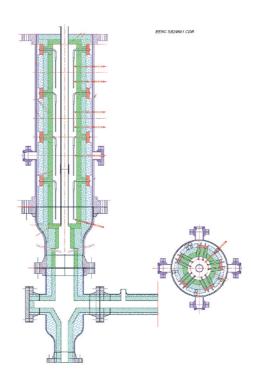


Figure 20: EERC's Entrained Flow Gasifier (EFG) photo/schematic.

Gasification of the petcoke in the EFG was not a trivial task. Petcoke is inherently unreactive and requires high temperatures to effectively gasify. The EFG unit was constructed in 2008/2009, so the EERC personnel were climbing a learning curve in its operation. Petcoke had never been fired in this unit before, representing another technological step out. The EFG is normally operated in slagging mode with most fuels (*i.e.*, low rank coals). Petcoke, however, has a rather high ash melt temperature which makes operation in this mode more difficult. Initial petcoke runs were targeted in the slagging regime resulting in several operational issues (plugging of the gasifier) and limited on-stream time. Limestone addition was also attempted to serve as flux and promote lower temperature melting of the slag, but the results were not very encouraging.

In the end, the decision was made to operate the gasifier at lower temperatures, below the ash melting temperature, and remove the spent petcoke as ash rather than melted slag. This helped reduce temperatures in the gasifier which led to improved on-stream time. High  $N_2$  purge flows were also adopted (at the expense of syngas purge flows) to help keep critical gasifier components (e.g., electrical junctions) at acceptable temperatures. The  $N_2$  introduced in this manner effectively diluted the sour syngas by about 50%, but was deemed necessary to maintain gasifier operability. Even with the lower temperature operation, the most

important aspect of these tests was preserved - the various sour syngas species that could become problematic in the PSA were still present, albeit at a lower partial pressure due to the dilution effect.

To date, a total of four campaigns have been attempted with the EFG/Sour PSA. A summary of the campaigns is contained in Table 6. Two of them have been successful, campaigns PC1 and PC4. Further details of the individual campaigns are outlined in the next section.

Table 6. Summary of EFG/Sour PSA campaigns.

Campaign	Dates	Feedstock/gasifier	Number of cycles
PC1	1/19 - 1/21 2010	Petcoke, EFG	225
PC2	2/22 - 2/23 2010	Petcoke + CaCO <sub>3</sub> , EFG	26
PC3	5/16 - 5/17 2010	Petcoke + CaCO <sub>3</sub> , EFG	5
PC4	5-24 - 5/28 2010	Petcoke + CaCO <sub>3</sub> , EFG, milder conditions	315

In total 570 cycles have been completed on the PSA to date with additional campaigns planned during Summer 2010 with the goal to complete as many or more cycles with the petcoke-derived syngas feed as were performed with the coal-derived syngas. Analogous to the coal-derived syngas campaigns, H<sub>2</sub>S breakthrough experiments will be performed throughout the campaign. The adsorbent capacity for H2S measured after PC1 is essentially the same as measured with the fresh silica gel. Once the campaign is completed, the columns will be removed and shipped to APCI for post-mortem analysis.

#### Campaign PC1

The gasifier was operated in slagging mode and 15 slpm of sour syngas was directed to the sour PSA unit. A total of 225 cycles were completed during this campaign. At cycles 125-130 samples of syngas were taken from the top (72" from feed end), middle (45" from feed end), and bottom (15" from feed end) taps in the bed. The results show essentially no H<sub>2</sub>S present at the top, 190 to 1300 ppm H<sub>2</sub>S at the middle port, and 1200 to 7400 ppm at the bottom port. The range of H<sub>2</sub>S at a particular spot is associated with compositions during the feed step (low levels) and regen steps (high levels). The data indicates that an adsorbed H<sub>2</sub>S front is developing in the column. More importantly, observation of the min and max levels of the H<sub>2</sub>S response with time can indicate if the adsorbed H<sub>2</sub>S zone is stable, or if it is moving up or down the bed (indicated by increasing or decreasing min and max values).

The temperature history plots during this time indicate that the beds swing from about 15 to 50C during the process cycle. The flow rate history plots shows that the feed and effluent flows are more or less consistent from cycle to cycle. The overall mass balance parameter, determined by taking the total volume of feed gas added

during a complete cycle divided by the sum of product, purge and depressurization gas volumes during that cycle, averaged out to 1.015 indicating flows are within 2% of expectation.

The min and max  $H_2S$  levels in the mid-bed history plots show a slow but continuous increasing trend, especially during the earlier cycles (Figure 21). It was felt that the beds were not being purged enough, in which case more  $H_2S$  is adsorbed during feed than can be removed by purging. This leads to eventual saturation of the bed, poor performance, and an inability to achieve cyclic steady state. To counteract this, the purge flow was increased at cycle 159. The impact on the mid-bed  $H_2S$  level was dramatic – increased purge more effectively cleaned the bed during regeneration, pushed the adsorbed  $H_2S$  zone towards the feed end of the bed, and lowered the  $H_2S$  min and max swings. The increased purge also slightly reduced the product gas flow rate, as expected since the purge source is taken from the product gas tank.

The PSA ran in this mode for an additional 47 cycles. At cycle 225 the PSA was shutdown because the EFG became unstable. Before this instability, a sample of the feed and product gas was taken in a stainless steel cylinder for chemical analysis.

Figure 22 illustrates the gas composition of the gasifier effluent gas, i.e., the PSA feed gas. It was obtained from a dedicated EERC GC. The compositions are rather steady until the end of the campaign. The gasifier nominally produced syngas containing 40% H<sub>2</sub>, 29% N<sub>2</sub>, 29% CO<sub>2</sub>, 1% H<sub>2</sub>S, 1% CO. Gas leaving the PSA was analyzed by a microGC in the sour PSA skid, and the results are plotted in the lower plot of Figure 22. Again, the compositions are initially relatively constant. The CO<sub>2</sub> composition decreases dramatically once the purge gas rate is increased, much like the H<sub>2</sub>S. Additional variability is evident during the latter stages of the campaign. The PSA produces gas nominally containing 65% H<sub>2</sub>, 34% N<sub>2</sub>, 0.04% CO<sub>2</sub>, 1% CO. Sulfur species H<sub>2</sub>S and COS are not observed, although the micorGC can only see those components at levels around 50 ppm or higher. Based on these results it is expected under commercial gasifier conditions (*i.e.*, 0.1-3% N<sub>2</sub> in syngas feed) the sour PSA H<sub>2</sub> purity will meet or exceed commercial application specifications.

The gas samples were pulled at a reasonably stable time period, although analysis of the performance of the PSA is somewhat ill-advised for this run as the PSA was never at a true cyclic steady state as evidenced by the observance of the increasing concentration of  $H_2S$  in the gas phase being sampled at the middle of the bed. Figure 21 shows the increasing  $H_2S$  front observed throughout this campaign. The cylinders were analyzed by Atlantic Analytical, and a report of their findings is attached in the Appendix B.

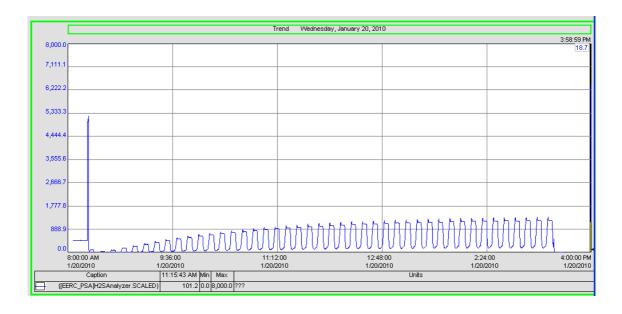


Figure 21. Gas phase H2S level (ppm) at middle of Bed A

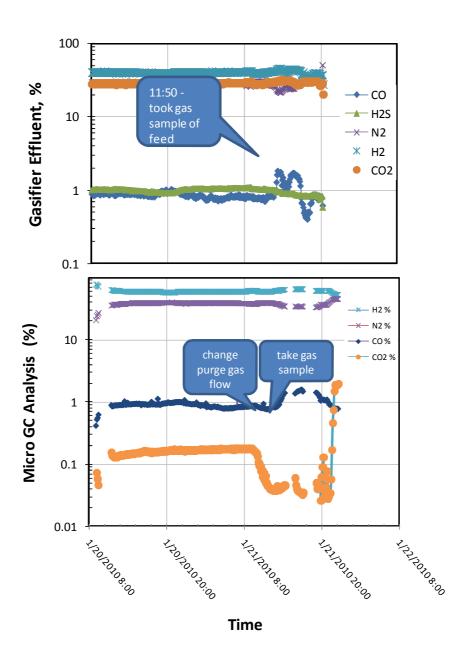


Figure 22. Gas composition of PSA feed gas (top) and PSA product gas (bottom)

A comparison of the various composition analyses for the major syngas components is presented in Table 7. There is rather good agreement between the EERC GC, the microGC, and the laboratory analysis of the gas cylinder samples for all the major components. The lab analysis also indicates that in addition to  $H_2S$  there is 15 ppm COS and even 1 ppm methyl mercaptan in the PSA feed gas. Unlike the CFBR tests, there is very little evidence of aromatic species, i.e., tar components, in the PSA feed. A trace amount of benzene (0.2 ppm) is the only aromatic detected. The lab analysis also detects 10 ppm ethane, 0.1% Ar and 0.17%  $CH_4$  in the PSA feed gas, which are generally not picked up by the other GC's. Lab analysis of the PSA product gas indicates low levels of  $H_2S$  (7 ppm)

exist – these are below the GC detection limits. There is no evidence of other sulfur species in the product gas. A separate test was conducted by the analytical lab to measure nickel or iron carbonyl in both samples. None of these materials were detected (limits of detection 5 ppm for nickel carbonyl and 1 ppm for iron carbonyl).

Table 7. Comparison of various gas compositions for the sour PSA feed and product gas.

	FEED			PRODUCT	
H <sub>2</sub>	41.7	39.8	38.8	60.3	62.0
N <sub>2</sub>	28.5	30.1	30.6	38.6	36.8
CO <sub>2</sub>	29.0	28.2	27.7	0.18	0.13
СО	0.67	0.80	0.76	0.69	0.86
CH <sub>4</sub>	0.17	0.08	ND	0.12	ND
AR	0.10	NA	NA	0.13	NA
H <sub>2</sub> S (ppm)	10550	10369	10200	7.1	ND
COS (ppm)	15	20		ND	ND
Methyl Mercaptan	1.5	NA		ND	NA
(ppm)					
Water (ppm)		300-500			ND
Ethane (ppm)	10	ND		ND	ND
Benzene (ppm)	0.2	NA		ND	NA

#### **Campaign PC2**

During this run the petcoke was spiked with CaO in order to help reduce the melt temperature and effectively operate the gasifier in slagging mode. Calcium oxide can react with H<sub>2</sub>S, COS and CO<sub>2</sub> via the following reactions:

- 1)  $H_2S + CaO = CaS + H_2O$
- 2)  $COS + CaO = CaS + CO_2$
- 3)  $CO_2 + CaO = CaCO_3$

Thermodynamic calculations were conducted with a system containing 10 atm of steam to determine the fate of  $H_2S$  and COS in the gasifier at 1500C. At this temperature the reverse of reaction 3 is favored, reaction 1 proceeds in the forward direction if the partial pressure of  $H_2S$  is greater than 0.13 atm and reaction 2 proceeds in the forward direction if the partial pressure of COS is greater than 0.02 atm. The partial pressures of  $H_2S$  and COS in the gasifier are anticipated to be greater than these limits, so the expectation is that CaO added will eventually form CaS. The amount of sulfur effectively removed was determined by simple mass balance assuming 0.25 lbs of CaCO<sub>3</sub> is added to every 25 lbs of pet coke. Roughly 5% of the available sulfur will be removed, which will not significantly impact the  $H_2S$  level in the sour PSA feed gas.

For this campaign, the PSA was operated for only 26 total cycles before multiple heating zones of the gasifier failed. Complete gasifier shutdown, and rather lengthy heater replacement and repair, became necessary. The gasifier was effectively down for a little more than two months.

#### Campaign PC3

The PSA was started up and 5 cycles were conducted, but the campaign was terminated early by failure of the oxygen/steam superheater system in the gasifier. This led to overheating of the process piping and oxidant feed header of the gasifier, necessitating complete cooldown of the gasifier for repair.

#### Campaign PC4

In this campaign, the decision was made to back down on the gasifier operating conditions to help extend its onstream time. Lower levels of oxygen would be fed, along with higher amounts of  $N_2$  purge.

Some modifications were also made to the PSA unit in preparation for this run. First, a galvanic  $H_2S$  analyzer was shipped from APCI and installed to provide dedicated analysis of ppm levels of  $H_2S$  in the PSA product gas. The continuous signal would permit more precise control of the PSA to achieve the desired goal of 2-5 ppm in the product gas. It also would enable better evaluation of process performance and comparison with simulations. The analyzer was zeroed and spanned with 10 ppm  $H_2S$  calgas before the run.

Second, two separate assemblies were constructed to help identify trace contaminants in the PSA feed and product gas. They consisted of a rotameter followed by two small sample tubes containing activated carbon and silica gel. One assembly was placed before the feed gas mass flow controller, and the other was placed directly off of the product tank. The idea was to continuously flow around 100 sccm of gas across the sample tubes, and then subsequently analyze the exposed adsorbents for trace species. Two different adsorbents were chosen to maximize the potential for capturing a variety of species. The columns were arranged in series, with the carbon column ahead of the silica gel column.

PSA cycles were started with petcoke derived syngas on May 24. As in PC1, the  $H_2S$  CEM was set up to monitor the  $H_2S$  level in the middle port of Bed A. After 21 cycles, the gasifier required shutdown due to a petcoke plug in the feed assembly, so the PSA was manually shut down.

Cycles resumed on May 25. The  $H_2S$  level in the product gas climbed rapidly during the next forty cycles, reaching ~9 ppm. After a quick check of the analyzer zero and span, action to reduce the  $H_2S$  level in the product was taken by reducing the feed rate (after a total of 64 cycles). This swiftly reduced the  $H_2S$  level in the product gas, and it hovered between 2 and 4 ppm for the remainder of the run. The min and max  $H_2S$  values from the mid-bed CEM also declined with the lower feed rate, and then stabilized.

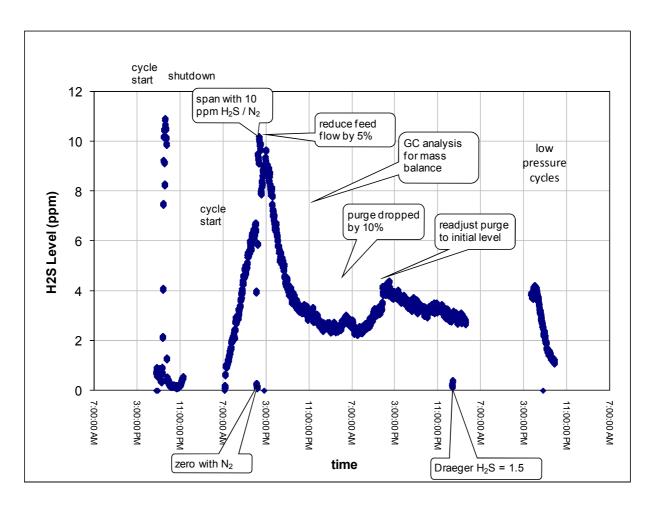


Figure 23. H2S Composition in PSA product gas determined by galvanic sulfur analyzer.

Once the  $H_2S$  level in the product gas appeared to stabilize, the microGC was used to analyze the composition of the feed, purge, and depressurization gases to allow for component mass balance estimates. The PSA then ran overnight at the same settings, although on two occasions the purge gas flow rate needed to be adjusted to bring the H2S level in the product gas back to the desired 3.0 ppm. On May 27 the gasifier experienced another petcoke feed issue as well as trouble with the syngas recycle compressor. The gasifier and the PSA were shutdown at 4:10 on May 27.

The recycle compressor was taken offline and found to require major repairs. Rather than stop all testing, EERC suggested running the EFB in a once-through mode, which does not require the recycle compressor. The highest pressure that can be achieved is limited to 250 psig by the gasifier. The PSA was adjusted to run 200 psig cycles, and a total of 25 process cycles were conducted. Unfortunately, at around 21:00 on May 27 the electrical feeds for the top gasifier heater shorted and the gasifier (and PSA) had to be shut down for good.

A total of 315 PSA cycles (equivalent to 53 hrs of run time) were completed in this campaign. Operating the gasifier at less strenuous conditions yielded improved on-stream time. The PSA was locked into a single set of

operating parameters for 227 of these cycles. The  $H_2S$  composition of the product gas was observed to stabilize and then remain relatively constant during these cycles. The PSA also responded as expected to changes in the purge flow. Although the PSA on-stream time was not extensive, the results show no evidence of a significant decline in performance over a 48 hr period. This is also evident in the product compositions for the other syngas components illustrated in Figure 24. These results are encouraging signs that the  $H_2S$  in the petcoke syngas can be effectively removed by the PSA.

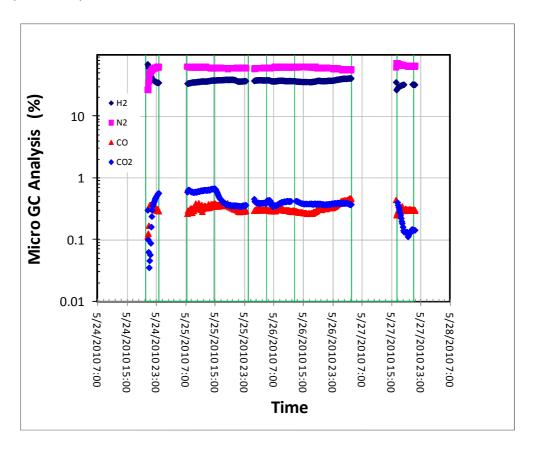


Figure 24. Gas composition of product gas (green lines correspond to transitions listed in Figure 23).

The compositions of the feed stream and the depressurization, purge, and product effluent streams are listed in Table 8 (derived from the GC shots taken on May 26). The results show that the sour PSA can effectively separate the acid gases from the other syngas components. In this run the PSA takes a syngas stream containing 7500 ppm  $H_2S$  and 23.5%  $CO_2$  and reduces the acid gas levels to 3 ppm  $H_2S$  and 4000 ppm  $CO_2$ . It was observed that  $N_2$  and CO pass through the column with little adsorption.

Overall PSA performance was determined from the composition data and total gas volumes collected from the feed mass flow controller and the dry test meters. The overall mass balance was within 3%. Component mass balances for  $H_2$ , CO,  $CO_2$ ,  $H_2S$  and  $N_2$  were also evaluated and found to be within 6%. The  $H_2$  recovery was 65%, significantly higher than in campaign PC1. Carbon rejection was 98.7% and the sulfur rejection was 99.98%. The **Air Products Confidential** 

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unique aspect of these results is that the PSA was at cyclic steady state when the analyses were conducted. Thus, these data can be compared directly with process simulations.

Table 8. Gas compositions for feed, depressurization, purge, and product gas streams.

	FEED	DEP	PURGE	PROD
H <sub>2</sub> , %	27.5	18.2	13.0	37.6
N <sub>2</sub> , %	47.8	40.7	24.0	60.6
CO, %	0.3	0.2	0.1	0.3
CO <sub>2</sub> , %	23.5	40.0	62.5	0.4
H₂S, ppm	7500.0	13200.0	21200.0	3.0

The galvanic analyzer on the feed gas was very useful in continuously monitoring PSA performance. There remains some concern, though, regarding the accuracy of the readings. At the end of the cyclic experiments the product gas  $H_2S$  level was measured with Drager tubes and found to be 1.5 and 2 ppm. The galvanic analyzer measured 3 ppm. A sample of the product gas was collected in a steel cylinder and will be tested by Atlantic Analytical to help resolve this discrepancy.

Simulations were conducted based on the experimental conditions of the sour PSA unit. The purge gas flow rate was fixed, and the feed flowrate was adjusted to achieve 3 or 6 ppm  $H_2S$  in the product gas. Comparison of the simulations with experimental data measured in campaign PC4 show the simulations over-predict the amount of product generated from the PSA, which leads to over-prediction of the  $H_2$  recovery by roughly 12 points. This is a rather large discrepancy and further work is necessary to understand its source. One possibility is failure of the multicomponent adsorption model to accurately predict the amount of  $H_2S$  adsorbed under multicomponent conditions (e.g., in large excess of  $CO_2$ ).

This is supported by the results of binary  $H_2S/CO_2$  breakthrough experiments. A series of breakthrough curves were conducted using 2.3% or 0.4%  $H_2S$  in He at 400 psig and 30 or 70C to calculate effective  $H_2S$  capacities. They are plotted in Figure 25 against isotherm model predictions at 30 and 70C, which were in turn based on experimental isotherm data measured for the same material with a volumetric isotherm unit. The breakthrough capacities are in excellent agreement with the isotherm model predictions, indicating that the latter can adequately describe the  $H_2S/silica$  gel equilibria for  $H_2S/He$  mixtures.

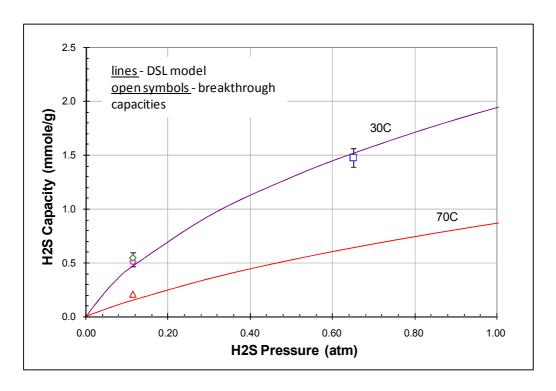


Figure 25. Comparison of Breakthrough Capacities with DSL Model Predictions for H<sub>2</sub>S in He.

Since  $CO_2$  and  $H_2S$  are rather strongly attracted to the adsorbent, the impact of  $CO_2$  on the adsorption of  $H_2S$  must be considered. This is particularly true for the feed gas to the sour PSA which contains on the order of 20 to 50 times the amount of  $CO_2$  as  $H_2S$  (e.g., 40%  $CO_2$  to 1%  $H_2S$ ).

A series of breakthrough experiments were conducted to measure the  $H_2S$  capacity in the presence of  $CO_2$  at 30C. The  $N_2$ -purged adsorbent bed was first completely saturated with a mixture of 30%  $CO_2$  in He at a total pressure of 400 psig. The feed gas was then switched to 10 slpm of gas containing various levels of  $H_2S$  (2.3%, 1%, 2000 ppm and 500 ppm  $H_2S$ ) in 30%  $CO_2$ , balance He. In this manner, the  $CO_2$  partial pressure remained constant throughout the entire experiment. Breakthrough of  $H_2S$  was monitored, and the effective  $H_2S$  capacity was determined from the stoichiometric breakthrough time and the feed flowrate.

The equilibrium  $H_2S$  capacities measured in this manner are presented as the red symbols/dashed line in Figure 26. These can be directly compared to the blue and brown lines corresponding, respectively, to the predicted capacities for pure  $H_2S$  (He is nonadsorbing) and  $H_2S$  in a 30%  $CO_2$ /balance He mixture. Both of these calculated curves were determined from our standard dual site Langmuir isotherm that we often use for describing multicomponent syngas adsorption. It is clear that the presence of  $CO_2$  has a very significant impact on the  $H_2S$  capacity (comparing the blue line to the other two). It is also evident that the isotherm model overpredicts the binary  $H_2S$  loading. This will yield optimistic numbers when the isotherm is used in process simulations (longer predicted breakthrough times than observed).

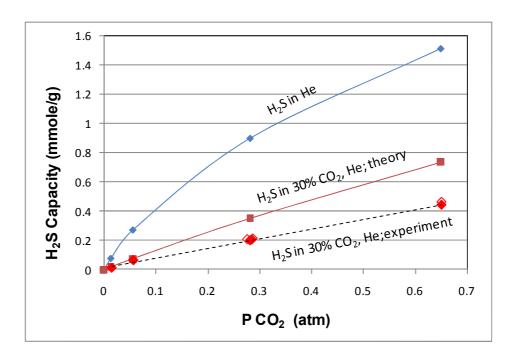


Figure 26. H<sub>2</sub>S capacity as function of H<sub>2</sub>S partial pressure in 30% CO<sub>2</sub>/He at 400 psig, 30C.

#### **Exposure testing**

As mentioned previously, a ten bed exposure test unit has been used in this work to determine the impact of  $H_2S$  on typical commercial adsorbents, and these results guided our selection of the material of choice in the PSA. In a final phase of testing, the most promising adsorbents were exposed to low levels of COS, HF, and  $Fe(CO)_5$  under various conditions for an extended period of time (~3 months). For these tests, the exposure unit was modified to address safety concerns (added dual valving to the columns, added CO in every feed gas to act as a leak detector). At this point in time, ten samples have been exposed for three months to 500 ppm COS, 500 ppm CO in  $N_2$  at 400 psig and a range of temperatures. The samples have undergone a color change, but the  $CO_2$  capacity of the materials remains similar to fresh adsorbents. The fully exposed materials will be removed at the end of May and thoroughly analyzed by xps to determine the composition of any deposited materials. Exposure with 50 ppm HF, 500 ppm CO in  $N_2$  is planned to begin in June, and the last series of tests with 10 ppm iron carbonyl, 0.25% CO in  $N_2$  is expected to begin in September. The results of this effort will allow for a better understanding of the potential deleterious effects of these species on the adsorbents.

Throughout the integrated gasifier/PSA testing, AP has derived great value from their relationship with EERC. Air Products has learned a great deal about the robustness and operability of the PSA in sour syngas operations. PSA model validation and reconciliation has also been achieved through the work conducted at EERC. During the testing, AP has found EERC to be accommodating and responsive to aide in the success of the experiments. Air Products looks forward to continuing their relationship with EERC.

#### Update Activity 3: Pre-FEED design of prototype. Risk analysis and mitigation.

AP will provide the required technical personnel to design the pre-FEED prototype. AP will perform a technical risk analysis and recommend a mitigation plan. AP uses a Technical Risk Management Process (TRMP) with risk quantification analysis, periodic multi-disciplinary functional reviews, an independent review with our Chief Engineer's office, development of new technology acceptance criteria (e.g., specific results required from a field demonstration unit, or R&D testing), and resolution of the technical risks. AP may choose to utilize the A&E coordinated by AERI in Activity 1. AP will review the results of Activity 3 with AERI.

Air Products has completed the high level assessment of the technical risks for the overall technology. Table 9 shows the overall technology subsystems and the relative risks. Air Products will continue with the technical risk assessment and mitigation plan, which include the following next steps:

- Risk quantification analysis
- Independent review with our Chief Engineer's office
- Development of new technology acceptance criteria (e.g., specific results required from a field demonstration unit, or R&D testing)
- Identification of fallbacks
- Review how the Activity 1 results (Jacobs study) impact the pilot design
- Leverage the knowledge from developments in Oxy-combustion/Sour Compression pilots.

Table 9. High Level Assessment of Main Technical Risks for pre-FEED Prototype

STEP-OUTS AND NEW TECHNOLOGIES	WHY IS IT A RISK?	WHY IS IT BEING TAKEN?
Use of H <sub>2</sub> PSA to remove H <sub>2</sub> S/CO <sub>2</sub> from gasifier syngas	A large scale H <sub>2</sub> PSA that removes high levels (%) of H <sub>2</sub> S has not been demonstrated	The H <sub>2</sub> S/CO <sub>2</sub> H2 PSA eliminates the upstream AGR (Rectisol/Selexol)
Use of H <sub>2</sub> PSA to remove trace levels of impurities (HCN, COS, etc.) from gasifier syngas	A large scale H <sub>2</sub> PSA that removes trace levels of solid fuel impurities (HCN, COS, etc.) has not been demonstrated	The H <sub>2</sub> S/CO <sub>2</sub> H2 PSA eliminates the upstream AGR (Rectisol/Selexol)
Oxy-combustion of tailgas	Oxy-combustion of sour PSA tailgas has not been demonstrated at scale	Oxy-combustion of the tailgas provides the CO <sub>2</sub> product
CO <sub>2</sub> purification system with acid removal	Has not been demonstrated at scale	Removal means for sulfur species

Complementary to the high level technical risk identification, Air Products has evaluated the key risks and unknowns associated with the technology which are currently being addressed or planned to be addressed in the near future. These include:

- 1) The stability of the adsorbents used in the PSA for sour gas applications
- 2) Differences in scale-up parameters from standard sweet H<sub>2</sub> PSAs and the new sour PSA.
- 3) The ability to maintain and control the oxy-combustion of the PSA tail-gas.

- 4) The reactor sizing and product compositions from the conversion of SO<sub>x</sub> into H<sub>2</sub>SO<sub>4</sub>.
- 5) How the operation and integration of the individual parts of the system will interact.
- 6) The fate of trace components that arise from the gasification process.

Testing has either been completed or is planned in the near future to address items 1, 3 and 4 using laboratory-scale equipment. Items 2, 5 and 6 require further investigation and a demonstration-scale unit which combines all the pieces of technology would be best suited to addressing these risks although testing of individual components of the system is also conceivable. Towards this end, Air Products has completed an initial assessment of the pilot to consider for the pre-FEED Prototype design. Table 10 lists some of the assumptions for the prototype.

Table 10. Initial Assessment of Pilot for the Design of the pre-FEED Prototype

Pilot Site Criteria for Advanced CO <sub>2</sub> capture system for sour syngas			
Assumption	Full System (Sour PSA, oxy-combustion, CO2 purification/compression)	Sour PSA only	
Overall Pilot Costs	CAPEX/ OPEX – TBD	CAPEX/ OPEX - TBD	
Site owner	Willingness to host pilot and provide support	Willingness to host pilot and provide support	
Pilot Scale	TBD; Nominally 0.1 to 10 mmscfd syngas feed; 3 to 300 tpd CO2	TBD; Nominally 0.1 to 10 mmscfd syngas feed	
Gasifier Type	Prefer large scale commercially available types (e.g., GE, others) and types that would match gasifiers that first adopter would utilize	Prefer large scale commercially available types (e.g., GE, others) and types that would match gasifiers that first adopter would utilize	
Feedstock	Petcoke, Coal, Heavy resids; prefer feedstock that first adopter would utilize	Petcoke, Coal, Heavy resids; prefer feedstock that first adopter would utilize	
% S in Sour Syngas	0.1 to 2.0% wgt; prefer % that first adopter would utilize; adjustable S% / species would be ideal	0.1 to 2.0% wgt; prefer % that first adopter would utilize; adjustable S% / species would be ideal	
Feeds / Utilities - Into pilot site			
Sour Syngas into site	>450 psia; nominally 0.1 to 10 mmscfd sour syngas	>450 psia; nominally 0.1 to 10 mmscfd sour syngas	
Power	Sufficient for system; kWh / V TBD	Sufficient for system; kWh / V TBD	
Oxygen	>99% purity, 50 psia; LOX if scale is right; otherwise ASU / P/L	N/A	
Boiler feed water	Yes; specs TBD	N/A	
Cooling Water	Yes; specs TBD	N/A	
Potable Water	Yes; specs TBD	N/A	
Fire Water	Yes; specs TBD N/A		
Nitrogen	Yes; specs TBD	Yes; specs TBD	
Instrument Air	Yes; specs TBD	Yes; specs TBD	
Effluents from pilot site			
15 bar acid condensate	Facilities to handle acid byproducts	N/A	
30 bar acid condensate	Facilities to handle acid byproducts	N/A	
Storm and Wastewater	Facilities to handle stream	Facilities to handle stream	
Return Cooling Water	Facilities to handle stream	N/A	
Vent from CO2 purification system	Permit allows vent	N/A	
Product quality CO2	Assume 30 bar unless pipeline home for higher pressure CO2 available; liquid CO2 byproduct???	N/A	
PSA tailgas	N/A	Facilities to handle stream (flare?)	
Product H2 (purity TBD)	Strong preference for site to utilize product H2 (at least fuel value)  Strong preference for site to utilize H2 (at least fuel value)		
Flare	Yes, sized for full trip	Yes, sized for full trip	

Miscellaneous		
Permitting	Any issues	Any issues
Time of pilot	6-18 months	6-18 months
Plot space	Available	Available
Host operators	Available	Available
AP global operations	Proximity to AP operations would be preferred	Proximity to AP operations would be preferred

Assuming the full system is to be demonstrated, the next step is to define the overall scope for the battery limit conditions for the prototype. A mapping of syngas feed rates versus the bed diameter of a ten bed PSA systems is shown in Figure 27. The mapping allows one to relate the size of the PSA to the syngas feed flow rate as well as an effective Net MWe from the hydrogen product. Also shown on the figure is the past experimental oxycombustion tests for the fired heater burner. It would appear that a 2' diameter PSA bed offers a reasonable scale up from the EERC work and would match well with the burner sizing. Table 11 shows the effective battery limits for a typical 2' diameter bed x 10 bed PSA system (with 97% CO<sub>2</sub> removal). Other factors for the design basis are shown in Figure 28 (Sour PSA) and Figure 29 (Sour combustor / Fired heater).

It was decided by the Technical Committee based on the results from Activity 1 to focus on:

- 1. Reduction of CAPEX and OPEX for the AP technology
- 2. Development of a Sulfur / Claus Gas alternative for the AP technology

Thus, further designs of the prototype were placed on hold in order to further develop these activities.

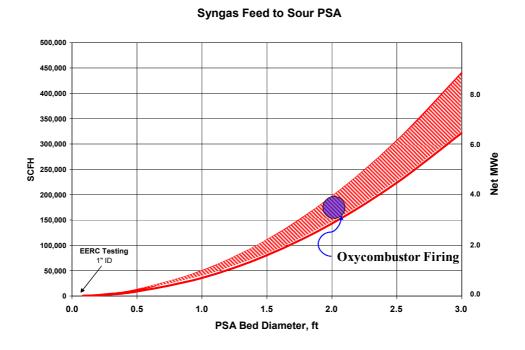


Figure 27: Map of Syngas Feed and PSA sizing.

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Table 11. Process Design Basis for typical 2' diameter bed x 10 bed PSA system (with 97% CO<sub>2</sub> removal).

	Range
Syngas Feed	140,000 - 200,000 scfh
	(3700 - 5300 Nm <sup>3</sup> /hr)
Net MW <sub>e</sub> (power cycle)	2.75 – 3.75 MW <sub>e</sub>
H <sub>2</sub> make (95% purity)	65,000-90,000 scfh
	(1700 – 2400 Nm <sup>3</sup> /hr)
Burnerfiring	4.0-5.5 MBtu/hr (million Btu/hr)
	(1.2-1.6 MW <sub>th</sub> )
O <sub>2</sub> for burner	0.36-0.49 stph
	(0.33-0.45 mtph)
CO <sub>2</sub> capture	3.9-5.3 stph
	(3.5-4.8 mtph)

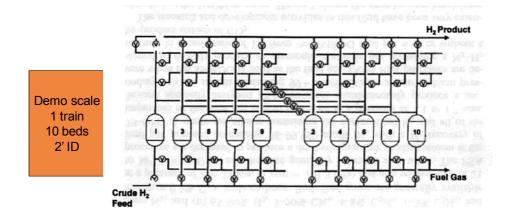
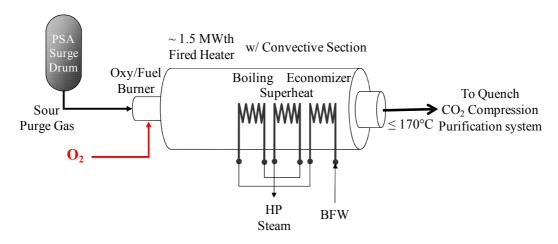


Figure 28: Proposed next scale Sour PSA sizing.



Design Considerations	Items to be Addressed
Fired heater plus convective surface area	Materials of construction (fired heater & convective coils)
Design to ≤ 170°C exhaust temperature	Acid dew point
Heater run slightly pressurized (150 mbar)	Control system
Sized to match Sour PSA (~1.5MWth fired heater)	Heat integration/utilization

Figure 29: Proposed next scale sour combustor sizing.

Based on the results of Activity 1 as well as discussions with the Technical Committee, Air Products has begun development of alternative sour gas treatment options for the Sour PSA tailgas. This study presents alternate sulfur-disposition options to AP's novel oxy-combustion/compression technology. The aim of this study is to expand potential flowsheet options involving the Sour PSA technology for carbon capture processes in sour syngas applications. It is expected that these flowsheet options will have capital and operating cost savings compared to the conventional technology as well as facilitate adoption of the Sour PSA technology by potential customers by providing additional flexibility in sulfur removal options.

To date, AP has completed a review of commercially available Sulfur disposition technologies and has screened them for potential applicability in the Sour PSA process. Work is underway to short-list the most promising options and perform detailed flowsheeting and costing analysis. The following table lists several potential S-disposition options and possible screening criteria for applicability in the Sour PSA process.

Sulfur Disposition Technology	Potential Screening Criteria
Upstream H₂S absorber (TSA) w/ Claus	CAPEX/OPEX savings w.r.t. conventional technology
Tailgas solvent w/ Claus	Commercially proven technology
Modified Claus Processes	
- CrystaSulf	Robustness to feed variation (composition/flow)
- Selectox	
Direct Oxidation (DO)/Redox Processes	
- LO-CAT	Product/By-product quality
- SulfaTreat-DO	
Alternative tailgas recycles/process integrations	Complexity/Reliability/Operability
Sour Combustion w/ FGD	
Thiopaq (biological)	

#### Update Activity 4: Select candidate sites in Alberta for demonstration plant. Identify and validate options.

AP will provide the required technical and commercial personnel to identify and visit candidate sites for the demonstration plant (up to four candidates). AP will coordinate with AERI to approach the relevant parties in Alberta in this regard. AP will then rank and assess the candidate sites in Alberta and review the ranking with AERI.

It was decided by the Technical Committee, given the current temporary slowdown in the status of gasification projects in Alberta, that selection of candidate sites was not prudent at this time. Those resources were reallocated to activity 2 (EERC experimental program) and further develop alternative sulfur disposition cycles as described in Activity 3. Future meetings with potential first adopters will proceed as possible.

#### Update Activity 5: Identify and qualify potential first adopters.

AP will provide the required technical and commercial personnel to identify and engage potential first adopters of the technology (up to three candidates). AP will coordinate with AERI to approach the relevant parties in Alberta in this regard.

It was decided by the Technical Committee, given the current status of gasification projects in Alberta, that qualification of first adopters was not prudent at this time. Those resources were reallocated to activity 2 (EERC experimental program) and further develop alternative sulfur disposition cycles as described in Activity 3. Future meetings with potential first adopters will proceed as possible.

#### Update Activity 6: Develop MOU with first adopter committed to build demonstration plant.

AP will provide the required commercial personnel to develop an MOU with a first adopter. AP will consult with AERI on aspects of the MOU and the siting of the demonstration plant.

It was decided by the Technical Committee, given the current status of gasification projects in Alberta, that selection of candidate sites and development of a MOU were not prudent at this time. Those resources were reallocated to activity 2 (EERC experimental program) and further develop alternative sulfur disposition cycles as described in Activity 3. Future meetings with potential first adopters will proceed as possible.

#### **Update Activity 7: Project Management.**

AP will provide the required project management. AP will provide status reports to AERI.

This report is the final scheduled status report to Alberta Innovates.

# Advanced CO<sub>2</sub> Capture Technology for Gasification of High-Sulfur Petcoke: Preliminary Feasibility Study of a Commercial Plant



**Prepared For** 

Air Products and Chemicals, Inc.

JACOBS Consultancy



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# Preliminary Feasibility Study of a Commercial Plant

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April 2009 Rich Hill

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# Appendix A JACOBS Consultancy

#### Section 1.



# **Executive Summary**

#### **JACOBS** Consultancy

Air Products, Inc. ("Air Products") is developing a new technology for processing the syngas resulting from the gasification of high-sulfur petroleum coke. The technology is designed to more efficiently capture CO<sub>2</sub> for sequestration, and as part of its product development, Air Products commissioned Jacobs Consultancy Inc. ("Jacobs Consultancy") to provide an independent opinion regarding the commercial feasibility of the technology. Two scenarios were evaluated: production of high-purity hydrogen for use in nearby refineries and chemical complexes, and net production of power. These scenarios were evaluated with Air Products' novel technology (hereafter referred to as Sour PSA), as well as with the conventional technology to provide a base case comparison. This report provides the preliminary plant conceptual design, performance, and capital and operating costs.

The comparative study focused on four cases:

- 1. GE Gasification followed by conventional technology to generate power while capturing CO<sub>2</sub>
- 2. GE Gasification followed by conventional technology to produce hydrogen while capturing CO<sub>2</sub>
- 3. GE Gasification followed by Sour PSA to generate power while capturing CO<sub>2</sub>
- 4. GE Gasification followed by Sour PSA to produce hydrogen while capturing CO<sub>2</sub>

The basis for the conceptual plant design is the target production of approximately 450 MW of net exported power for the power generation base case, adjusted to 453 MW to match turbine capacity, which gives a petcoke feed rate of 4,473 MTPD. The hydrogen production cases were developed based on the same petcoke feed rate.

Air Products' technology consists of the following novel components:

- Sour pressure swing adsorption (PSA) for hydrogen separation
- Sour oxy-combustor for the PSA tailgas
- Staged compression with conversion of NO<sub>x</sub> to HNO<sub>3</sub> and SO<sub>2</sub> to H<sub>2</sub>SO<sub>4</sub> and removal as waste acid streams

As mentioned above, in both the conventional and the Sour PSA cases, the gasification complex is designed to capture and compress the  $CO_2$  generated. The amount of carbon recovery to the sequestration-grade  $CO_2$  stream via the tailgas treating system varies by case, with 90% carbon recovery in the Conventional Power Generation Case, 95% carbon recovery in the Conventional

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Hydrogen Production Case, 91% carbon recovery in the Sour PSA Power Generation Case, and nearly 100% carbon recovery in the Sour PSA Hydrogen Production Case. Note that the recoveries for the Sour PSA cases would be decreased by 2-3% with the addition of acid neutralization.

For the Sour PSA, the general process scheme is as follows: Petcoke is fed to a conventional GE gasifier. The produced syngas undergoes shift conversion and cooling. The shifted gas is routed to a sour pressure swing adsorption (PSA) unit to recover a high-purity hydrogen product and a sour tail gas stream. The sour PSA tailgas is burned in an oxy-combustor to generate super heated steam for power generation in a steam turbine (existing in the combined cycle power block). The oxy-combustor flue gas is compressed in stages, resulting in the conversion of SO<sub>2</sub> and NO<sub>x</sub> to sulfuric acid and nitric acid, respectively, for removal. After removal of the other acid gases, the resulting flue gas is a concentrated CO<sub>2</sub> stream suitable for deep saline sequestration. A small fraction of the CO<sub>2</sub> stream is used as a diluent in the gas turbine for the Sour PSA Power case, and the remainder is compressed before exiting battery limits. The hydrogen that is separated in the PSA can either be consumed in a conventional combined cycle power block to produce power or as a high purity hydrogen stream for use by an upgrader, refinery or chemical plant.

For the conventional flowschemes, the configuration is the same through the production of the shifted syngas. Following the sour shift, a conventional two-stage Rectisol unit is used to remove the H<sub>2</sub>S and CO<sub>2</sub>. The resulting clean gas can then be used to produce hydrogen via a conventional PSA, or combusted in a conventional combined cycle block to produce power. The H<sub>2</sub>S and CO<sub>2</sub> are removed during the regeneration of the Rectisol. The H<sub>2</sub>S is converted to sulfur in a conventional sulfur recovery unit, and the CO<sub>2</sub> is compressed for sequestration.

Figures 1-1 through 1-4 are block flow diagrams of the process scheme for each of the four evaluated cases.

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Figure 1-1.
Block Flow Diagram: Air Products' Technology—Hydrogen Production

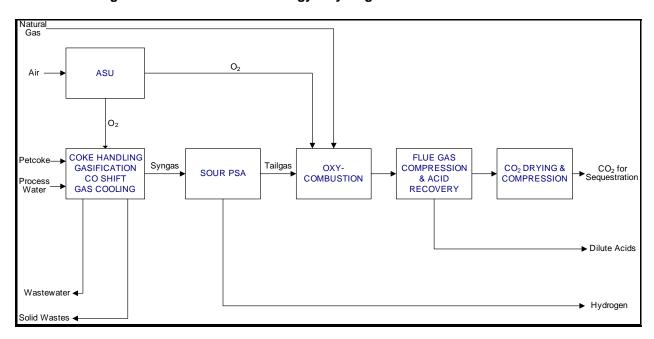
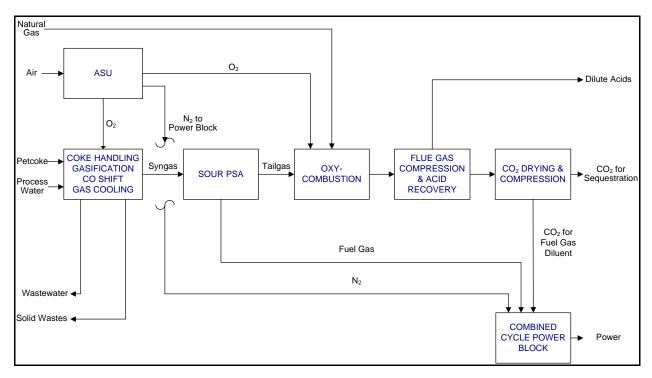


Figure 1-2.
Block Flow Diagram: Air Products' Technology—Power Generation



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Figure 1-3.
Block Flow Diagram: Conventional Technology—Hydrogen Production

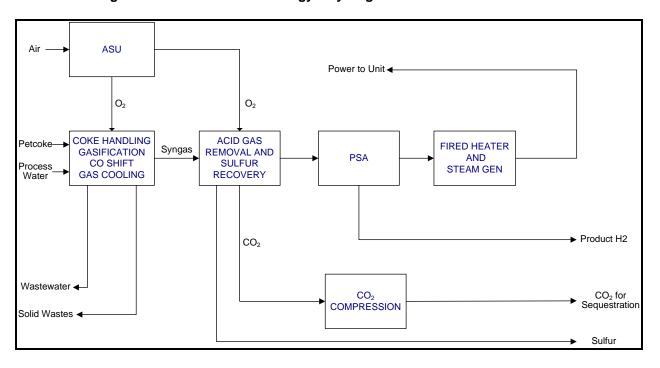
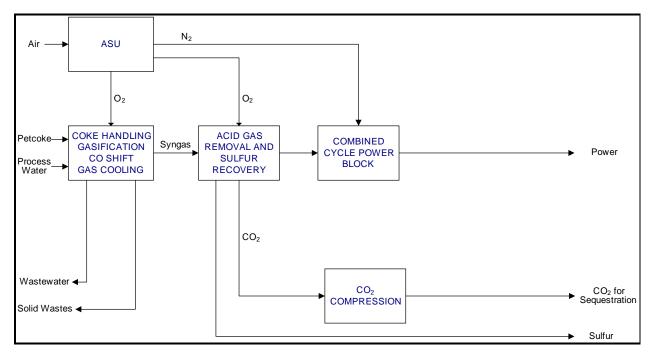


Figure 1-4.
Block Flow Diagram: Conventional Technology—Power Generation



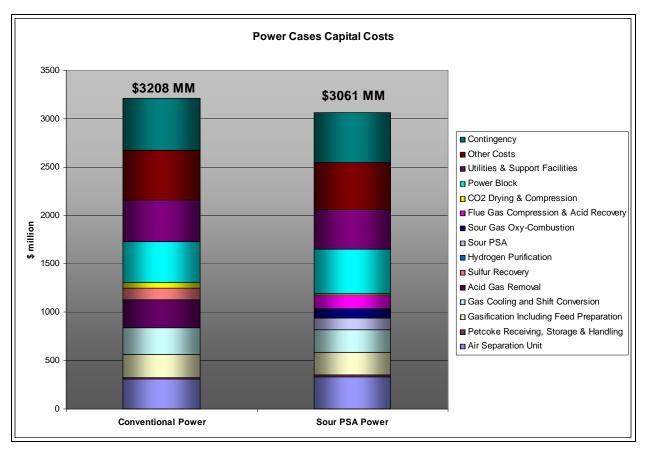
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# Appendix A JACOBS Consultancy

#### **Capital Costs**

Based on our review of the capital costs, the Sour PSA technology has the potential to reduce capital costs for both the hydrogen and power case on a standalone basis by \$110 to \$150 MM on a total investment of around \$2,600 to 3,100 MM. Although the savings are well within the accuracy intervals of the estimates (±50%), we can compare the mid-point costs for each case. Figures 1-5 and 1-6 below summarize the mid-point costs for each case.

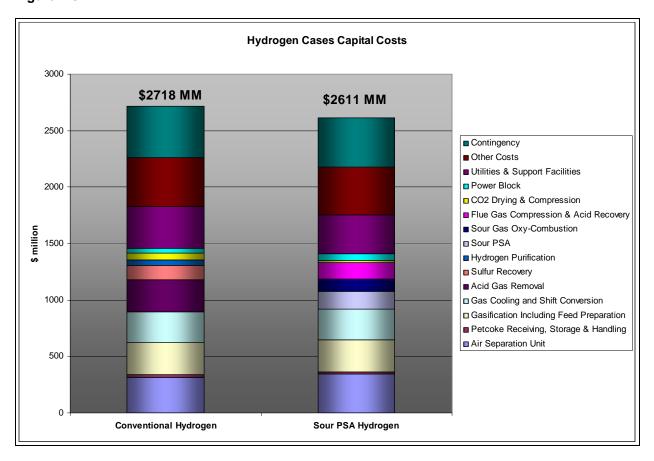
Figure 1-5.



The savings for the Sour PSA in the power case are about \$150 MM.

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Figure 1-6.



Note: The Acid Gas removal costs include compression up to 30 bar for the Sour PSA cases

The capital cost savings for the Hydrogen case are smaller than the Power at roughly \$110 MM. This is primarily due to the more expensive Sour PSA equipment required for the Hydrogen Case. However, it should be noted that the savings we show for the Sour PSA cases represent only about 4 to 5% of the total costs and are well within the noise of the estimates, which is ±50 percent. While the range of uncertainty in the actual costs should be the same for each case, the actual costs for constructing new technology are often skewed toward the high side of original estimates.

Furthermore, the savings could be much less for gasification plants that are situated near upgraders or refineries. In these situations, incremental investment in existing sulfur units would be substantially cheaper than a dedicated sulfur plant for gasification block, and would therefore reduce the capital costs for the conventional technology. For these reasons, we opine that an important aspect of the technology development program should be aimed at further reducing the capital costs.

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Key drivers for the capex reduction in both the Hydrogen and Power Sour PSA Cases vs. the Conventional Cases are as follows:

- Elimination of the entire Rectisol unit
- Elimination of the Sulfur Recovery unit
- Other factored expenses and contingency

Despite the elimination of these components, there are important cost considerations for the Sour PSA technology, including:

- Sour PSA system
- Sour Oxy-Combustor plus a larger ASU to provide high-purity oxygen
- Compressor equipment in the acid removal section requiring enhanced metallurgy

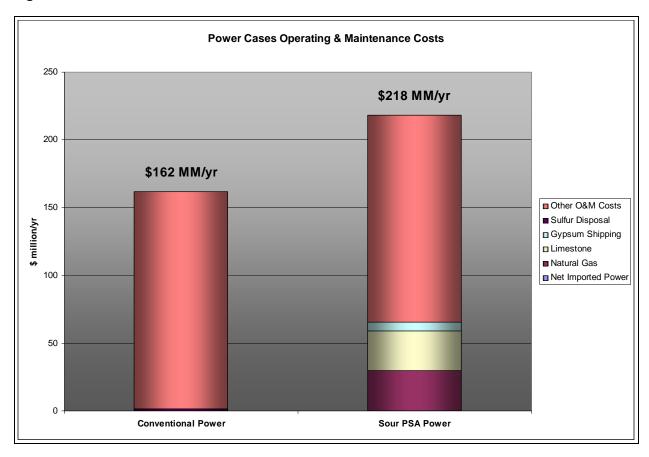
#### **Operating Expenses**

Based on our estimates of the operating expenses, the Sour PSA technology appears to have higher operating expenses primarily due to the acid neutralization costs. In addition to capital cost considerations, alternatives for the disposition of the sulfur-related compounds should be considered. The sulfuric acid production is anticipated to be relatively dilute and contaminated with some nitric acid. In addition, even in a pure state, the sulfuric acid volume is large relative to the market size.

Our preliminary market analysis indicates that the sulfuric acid production from this single preliminary design would be enough to supply the whole Western Canada market, and represents nearly 1% of the total North American market. Therefore, we expect that the acid would have to be neutralized and the resulting gypsum landfilled. Total costs for this are expected to be \$33,000,000 to \$40,000,000/yr, putting the Sour PSA at a distinct operating cost disadvantage relative to conventional technology which produces about 100,000 MT/yr of sulfur that, if not sold, can be readily stored safely and indefinitely. Figures 1-7 and 1-8 below summarize the operating costs for the Power and Hydrogen cases.

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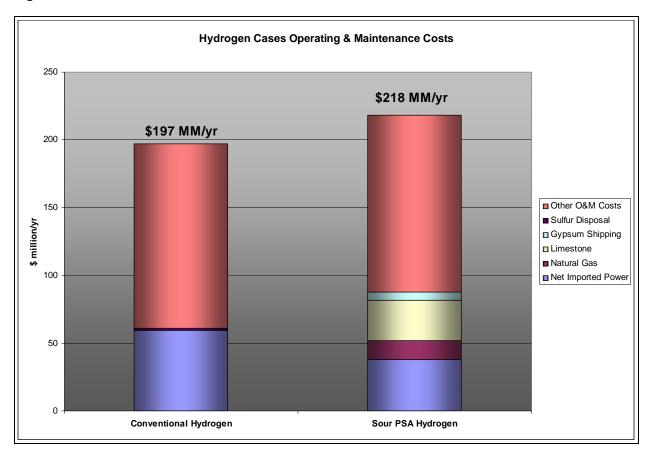
Figure 1-7.



In the Power case comparison, the operating costs for the Sour PSA case are roughly \$60 MM/yr higher due primarily to the neutralization costs as well as the incremental natural gas required for the Sour Oxy-Combustor.

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Figure 1-8.



In the Hydrogen case comparison, the operating costs for the Sour PSA case are only about \$20 MM higher with the neutralization costs offset by a reduction in the power required.

#### **Major Risks**

Any new technology has risks, especially early in the development program. One of the key issues to address for success is to understand the risks, develop mitigation strategies and potentially refocus efforts if potential "show stoppers" exist. For Air Products' Sour PSA technology, the key risks refer to the acid generation and removal and are listed as follows:

#### **High Acid Neutralization Costs**

Early in the study, acid disposal costs were noted as a potential risk. During the course of the study, we concluded that neutralization was the mostly likely disposal route for the dilute acid,

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and was therefore included in the operating costs. Due to the costs of neutralization, there may be an incentive to produce a more concentrated sulfuric acid stream or identify less expensive disposal options. Air Products currently estimates that the sulfuric acid generated in the first stage will be dilute (40%-80%) and may contain some nitric acid as well. Although some potential offtakers of sulfuric acid (largely phosphoric acid plants associated with fertilizer production and, to a smaller extent, refiners and wallboard manufacturers) can accept lower purity sulfuric acid (perhaps down to 70%), we do not know of any long range transportation occurring at concentrations below 93% due to corrosion concerns.

Acid concentration issues aside, the current sulfuric acid market may be a constraint. This single application of the Air Products acid production would likely swamp the sulfuric acid market in Western Canada, which is currently around 300,000 MT/yr (dry) and represents nearly 1% of the total North American market. Therefore, just producing a more concentrated and contaminant-free sulfuric acid stream may not improve the marketability of the acid.

#### **Alternative Sulfur Removal Technologies**

A natural outcome of the difficulties associated with sulfuric acid production is to identify and consider alternative means of sulfur removal. A side benefit of an alternative scheme would be a reduction in the capital cost associated with the acid removal equipment including compressors, all of which require enhanced metallurgy to combat the corrosive environment associated with acid production.

#### Recommendations

Jacobs Consultancy opines that if the Sour PSA technology performs as claimed by Air Products, there may be small but significant capital cost savings associated with eliminating the Rectisol (or Selexol) system and the sulfur recovery unit, and adding in the Sour PSA, Oxy-Combustor and Acid Removal steps. Additionally, the Sour PSA power case produces significantly more power (20 MW) than the conventional case, increasing potential revenue for the power case. The Sour PSA hydrogen case, however, produces about the same amount of hydrogen as the conventional case. Despite the capital cost benefits and production benefits, at least for the power case, significant challenges exist with respect to operating costs, largely associated with acid production and uncertainty in the capital costs associated with new equipment. Key aspects in improving Air Products' capital and operating costs while maintaining performance include:

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#### Further reduction in capital costs:

Despite the elimination of two entire systems in the conventional flowschemes, the additional cost associated with the Sour PSA equipment including the Sour PSA, the Sour Oxy-Combustor and the Acid Production and Removal system provide modest cost reductions that represent 4 to 5% of the total cost of the entire gasification system. However, this capital cost advantage is less if the Sour PSA technology is evaluated in an industrial application where incremental sulfur capacity could be added relatively inexpensively to an existing sulfur plant associated with an upgrader or refinery.

#### Reduction in operating expense:

The operating expenses of the Sour PSA system are much higher than the conventional system due to the costs of neutralization and disposal of the sulfuric acid, which total approximately \$36 MM/yr.

#### Alternative means of sulfur component removal:

Identification and development of options related to removal of the sulfur components in the Sour PSA tailgas would reduce the operating expenses and may reduce the capital costs. Some options include PSA advancements, such as two-stage systems that would remove H<sub>2</sub>S as well as hydrogen, and compression and co-injection of H<sub>2</sub>S and CO<sub>2</sub> into sequestration wells.

#### Sour PSA performance

The Sour PSA system must be robust enough to separate the hydrogen from the shifted sour gas without overly contaminating the hydrogen stream or losing a significant amount of hydrogen to the tailgas. The system must be capable of meeting the performance requirements despite changes in the feedstock occurring through gasifier feedstock variability as well as operational changes.

# Appendix A JACOBS Consultancy

#### Section 2.



# Introduction, Scope and Objectives

#### **JACOBS** Consultancy

Air Products and Chemicals, Inc. ("Air Products") has developed an alternative CO<sub>2</sub> capture technology for use with conventional gasification technologies. Jacobs Consultancy Inc. ("Jacobs Consultancy") was retained to perform a commercial feasibility study of the process.

The study's focus is as follows:

- Development of high-level block flow diagrams with key process parameters for four cases:
- Two conventional technology cases
- Two Air Products technology cases
- High-level hazard identification of the alternate process
- Capital cost estimates
- Operating cost estimates

Jacobs Consultancy's role has been to assist Air Products in assessing the technical and economic feasibility of a conceptual commercial plant. Both scenarios—hydrogen production and power generation—have been evaluated with Air Products' novel technologies as well as the base case design, using conventional technologies, for cost and process comparison.

The scope of work provides the following technical and cost deliverables for the plant:

- Design basis
- Process & heat integration study
- Block flow diagram
- Heat & material balances for block flow diagram
- Hazard identification (HAZID)
- Emissions and flows at Battery Limits
- Utility Estimate / Plant Efficiency Evaluation
- Preliminary capital cost (CAPEX) estimates (± 50% accuracy)
- Operating cost (OPEX) estimates (± 50% accuracy)

# Appendix A JACOBS Consultancy

### Section 3.



## **Design Basis**

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#### Introduction

This design basis establishes the technical basis to perform a preliminary feasibility evaluation of a conceptual commercial plant that will produce high-purity hydrogen or generate power via the gasification of petroleum coke with novel CO<sub>2</sub> capture technology.

#### **General Criteria and Philosophy**

#### **Process Technologies**

There are several commercial gasifier licensors; however, for the purposes of this study, Jacobs Consultancy and Air Products agreed upon the GE quench technology. When a plant is to be designed, a formal licensor evaluation will be conducted that includes input from selected licensors on performance, cost, experience, commercial, legal and other issues.

Downstream of the gasification unit and water gas shift (shift) conversion section, Air Products' novel technologies are utilized. The effluent from the shift reactor is passed to a novel sour pressure swing adsorption (PSA) unit to recover a high-purity hydrogen product. The purity of the hydrogen product stream is determined by whether it is to be used as a hydrogen product for export, or as a fuel gas stream to a power block. The sour PSA tailgas is burned in a sour gas oxy-combustor, which produces heat that can be used to superheat steam for power generation in a steam turbine. The oxy-combustor product is compressed in stages, with cooling after each stage resulting in the condensation of water vapor in the tailgas stream.  $NO_x$  and  $SO_2$  in the tailgas react in the aqueous phase to form sulfuric and nitric acid, respectively. The acidic aqueous solution is removed and either processed for sale or disposed. The resulting concentrated  $CO_2$  stream is dried and compressed further and exported for sequestration.

For the conventional cases, the selection of technologies downstream of the gasification unit has been made based on previous experience and engineering judgment; the Rectisol process has been selected for acid gas removal. The degree of detail presented for licensed units is limited to non-confidential information.

#### **Feedstock and Products**

#### **Coke Properties**

Petroleum coke is used as feedstock for the plant. The feed rate, determined by fuel gas requirements for the selected gas turbine for the conventional power case, is 4,473 MTPD.

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Coke is fed to the gasifiers at a slurry concentration of 63 percent. Typical properties of the feedstock are provided in Table 3-1.

Table 3-1.

Typical Fuel Analysis for Petroleum Coke Feedstock

Proximate A	nalysis	Ultimate Analysis (d	ry basis)
Component	% By Weight	Component	% By Weight
Moisture	12.0%	Carbon	85.40
Volatile Matter	9.5%	Hydrogen	3.60
Fixed Carbon	74.6%	Sulfur	6.30
Sulfur	5.8%	Nitrogen	1.40
Ash	2.2%	Oxygen	0.80
		Ash	2.50
		Total	100.0
Heating Value		Petroleum Coke as Received	
BTU/lb (HHV)	14,620	Moisture (by weight %)	12.0%

#### **Oxygen Properties**

The plant will include a cryogenic Air Separation Unit (ASU) providing oxygen to the gasifier as well as to the Oxy-Claus sulfur recovery unit (base cases) and the sour oxyfuel combustor (Air Products cases). The produced oxygen feed will meet the specification in Table 3-2 below.

Table 3-2.
O<sub>2</sub> Purity / Specifications

O <sub>2</sub> Specification	Limit / Basis
O <sub>2</sub> (Power Generation Cases)	95 %
O <sub>2</sub> (H <sub>2</sub> Production Cases)	99.5%
Pressure to Gasifier	78 bar
Pressure to Oxyfuel Combustor	2 bar

#### **Hydrogen Product**

The hydrogen produced by the plant for export via pipeline will meet the specifications shown in Table 3-3.

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Table 3-3. H<sub>2</sub> Purity / Specifications

H <sub>2</sub> Specification	Limit / Basis
H <sub>2</sub>	≥ 99.99%
Total CO + CO <sub>2</sub>	≤1 ppm
Temperature	Process (44°C)
Pressure	Process (64 bar)

#### **Design Carbon Removal and Capture**

In all four cases, the plant is designed to economically capture the bulk of the  $CO_2$  generated from the plant. The additional capital cost and power consumption associated with  $CO_2$  capture and compression are included for all four evaluated cases. Other costs—including  $CO_2$  pipeline and sequestration costs—are not included but would be similar for each case.

The carbon recovery specification is based upon the total carbon ( $CO + CO_2$ ) from the gasifier outlet that is recovered in the  $CO_2$  product stream. Table 3-4 shows the total carbon recovery (based on  $CO + CO_2 + CH_4$  in syngas exiting the gasifier) for each case. The recovery is defined as carbon in the  $CO_2$ -for-sequestration product stream, from carbon at the outlet of the desaturator for the Conventional Cases, and across the Sour PSA to the PSA tailgas stream for the Sour PSA Cases. It is likely that the acid generated in the sour PSA cases will have to be neutralized for disposal. The most economic means of neutralization is through the use of limestone, which will release  $CO_2$  in contact with the acid. This will decrease the  $CO_2$  recovery by less than 2% and is not included in the  $CO_2$  recovery estimated for each case.

The quality of the  $CO_2$  was agreed upon by Jacobs Consultancy and Air Products for sequestration in deep saline aquifers based upon specifications in similar projects. Table 3-4 summarizes the  $CO_2$  purity specifications.

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Table 3-4. CO<sub>2</sub> Purity / Specifications

CO <sub>2</sub> Specification	Limit / Basis
CO <sub>2</sub> Purity	≥ 95%
Temperature	Supercritical
Pressure	≥ 2,200 psig
Total Non-condensable gases (N <sub>2</sub> , H <sub>2</sub> , Ar)	≤3-5%
H <sub>2</sub> S	≤150 ppmv
Carbon Recovery by Case	
Conventional Hydrogen Production	95%
Conventional Power Generation	90%
Sour PSA Hydrogen Production	99.9999%
Sour PSA Power Generation	91%

#### **Sulfur Recovery By-Product Specification**

For the Sour PSA cases, the initial  $CO_2$  compression new technology utilized in the plant design will provide the conditions to convert the  $SO_2$  to dilute sulfuric acid for removal. Due to the following factors, we opine that the acid will be neutralized with limestone and the resulting gypsum will be landfilled.

- The Air Products technology is likely to produce a sulfuric acid composition less than the 93% purity required for transportation.
- Based on the current sulfuric acid market according to published sources, this single application for the study basis would swamp the entire western Canadian market of about 300,000 MT/yr on a dry basis.
- Commercial concentration mechanisms are costly to build and operate, and are not competitive in comparison to elemental sulfur to sulfuric acid plants.
- There is an abundance of local sulfur supply due to the large oil sands operations in Alberta; therefore, raw material costs for elemental sulfur plants are very low.

For the conventional cases, the H<sub>2</sub>S will be removed in the Rectisol process and converted to sulfur in a conventional Claus sulfur removal unit.

The following specification is typical for traded liquid sulfur:

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• Sulfur purity (dry basis) >99.9 wt%

Color (solid sulfur) bright yellow

Inorganic ash
 250 ppm wt

Acidity
 100 ppm (as H<sub>2</sub>SO<sub>4</sub>)

Carbon
 250 ppm wt

• H₂S 10 ppm wt

### **Environmental Constraints**

### **Atmospheric Emission Limits**

The new technology utilized in the plant design includes a high-recovery  $CO_2$  capture. In the process,  $SO_2$  and  $NO_x$  are converted to sulfuric and nitric acid, respectively, and can be separated from the other tailgas products. The atmospheric  $SO_2$  and  $NO_x$  emissions will be minimal.

In the conventional cases, sulfur is removed as H<sub>2</sub>S to the Claus unit. Claus tailgas is recycled to the Rectisol unit, so there are essentially zero sulfur emissions from the Claus unit.

### **Liquid Discharge**

Liquid discharge will result from the gasifier wastewater, cooling water blowdown, and steam system blowdown.

### **Solids Discharge**

Spent catalysts or absorbents that cannot be reclaimed and sludge from the water treatment unit are treated as hazardous wastes and will be hauled away to a disposal site. These will be treated as an operating cost.

Coarse and fine slag from the gasifiers is non-hazardous and can be used for road making, construction, and landfill covering. The slag may therefore be considered a by-product rather than a waste stream.

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From a comparative standpoint, the main difference in solids discharge is that sulfur is produced in the conventional cases and gypsum is produced in the Sour PSA cases. Shipping and disposal costs are included in the operating costs for each.

### **Process Design**

### **Availability and Spares**

For the hydrogen cases, one spare gasifier train shall be included. For the power cases, no spare gasifier shall be provided.

All rotating equipment in the syngas treatment plant (except compressors, steam and gas turbines and generators) have installed spares on a "plus one" basis, *i.e.*, one 100% pump has a 100% spare; two 50% pumps have one 50% spare.

Major rotating equipment items such as the ASU air compressor are not spared.

All new units are designed for an operating life of 30 years.

### **Equipment Design Criteria**

Applicable US standards and codes such as ASME, API, BS, CSA and ISA were used in this study.

### **Site Information**

### Location

The proposed location is a greenfield site in Alberta, Canada. Edmonton was used as a location basis for cost estimating, assuming an industrial heartland location.

### **Miscellaneous Design Data**

Table 3-5 summarizes miscellaneous design criteria.

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Table 3-5. Miscellaneous Design Criteria

	Proposed Site
Mode of Coke Delivery	By conveyor from adjacent storage yard
Solids Disposal	Offsite disposal by truck or rail
By-Product Sulfur Transportation	By truck or rail
Live (Enclosed) Coke Storage	5 days
Sulfur Storage	5 days
Flaring During Start-Up	Assume that flaring of un-desulfurized syngas is acceptable during start-up so that a start-up AGR absorber is not required
Start-Up Fuel	Assume natural gas is available for start-up of gasifier and sulfur recovery unit

### **Definition of Battery Limits**

For the purpose of the study and cost estimates, the Battery Limits are defined as coke delivery from the conveyor, high voltage side of electricity supply, raw water and natural gas pipe inlet flanges, waste water pipe outlet flange, and the hydrogen and compressed carbon dioxide pipe discharge flanges.

### **Utilities**

### **Imported Utilities**

The site is considered to be greenfield. The following utilities are required at the battery limit of the plant:

 Raw Water—Raw water will be available at the plant battery limits for producing demineralized water, utility water, cooling water make-up, etc. Any limitations on raw water consumption will be determined during permitting.

Raw water supply conditions:

Maximum pressure	60	psig
Normal pressure	45	psig
Minimum pressure	30	psig

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- Natural Gas—Natural gas is available for start-up and for minor ongoing use as a support fuel in the sour PSA tailgas combustor at the battery limits.
- Power—There is a net power consumption in both the conventional and Sour PSA hydrogen cases. Power is assumed to be available at the battery limits.

### **Utilities Generated**

The following utilities are assumed to be generated:

- Cooling Water
- Steam—Steam is generated at high and low pressures.
- Power—There is a net power production in the Conventional Power Generation and Sour PSA Power Generation Cases, and power is exported in these cases.

# Appendix A JACOBS Consultancy

### Section 4.



# **Process Integration & Case Selection**

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To select the two flowschemes highlighting the Air Products technology, Jacobs Consultancy held an internal brainstorming session to identify various options available. These ideas primarily involved using heat integration within the process to maximize the power and heat generated by the configuration. The ideas generated internally were evaluated and ranked based upon the following criteria:

- Specific applicability to the novel technology cases—Ideas that pertained to the
  upstream gasification, gas shift, and cooling sections were not considered for this
  evaluation, since they would not differentiate the Air Products technology cases from the
  base cases.
- Value added to the process—Ideas were ranked high, medium, or low based upon the approximate benefit they would provide.

The most highly-ranked ideas from the Jacobs Consultancy internal brainstorming session were as follows:

- Increased sour PSA tailgas pressure to reduce compression costs; trade-off is lower recovery within the PSA and higher pressure oxyfuel combustion
- Wet limestone scrubbing of oxy-combustor flue gas
- Mercury removal before the Sour PSA or membrane WESP (claims to remove Hg)
- Use of the oxyfuel combustor heat to superheat steam at various pressures rather than making only saturated steam
- Use of a condensing economizer after oxy-combustor convection section to recover heat
- Use of an O<sub>2</sub> scavenging bed to remove inerts from CO<sub>2</sub> rather than using cold box (if inert removal is required)
- Neutralization and landspreading / landfilling of dilute acids
- Development of a design for less stringent sequestration specs, not for Enhanced Oil Recovery (EOR)

Starting with the most highly-ranked ideas from the internal brainstorming session, Jacobs Consultancy and Air Products identified other options for review and selection. The additional ideas were as follows:

Elimination of the cold box—no inerts removal

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- First stage of compression upstream of the oxyfuel combustion
- Other uses for acids (fertilizer, ammonia, etc.)
- Use of ash from a nearby power plant for acid neutralization (conventional pulverized fuel power plant)
- Use of the low-grade heat generated in the oxy-combustor and gasification sections for acid concentration
- Two-stage PSA: first stage CO<sub>2</sub> rejection, second stage for H<sub>2</sub> purity
- Two-stage PSA: first stage H<sub>2</sub>S removal to Claus unit, second stage for H<sub>2</sub> purity
- Two-stage PSA: Within an upgrader, use the first PSA to achieve the power block feed composition (within the H<sub>2</sub>S limits), and the second PSA to get product H<sub>2</sub> purity
- Purge the PSA with CO<sub>2</sub> instead of H<sub>2</sub> for higher CO<sub>2</sub> purity
- Purge the PSA with N<sub>2</sub>
- Licensed ammonia scrubber technology to convert SO<sub>2</sub> to ammonium sulfate for fertilizer
- Licensed technology to treat the flue gas by converting SO<sub>2</sub> to concentrated, high-purity sulfuric acid and converting NO<sub>x</sub> to N<sub>2</sub>

The complete list of ideas generated from the Jacobs Consultancy internal brainstorming session and Jacobs Consultancy / Air Products meeting can be found in Appendix 1.

Selection of the two Air Products technology flowschemes was based upon voting by the Air Products team members on all the ideas listed above: the highly-ranked options developed in the internal brainstorming session and the additional ideas identified by Jacobs Consultancy and Air Products. Criteria used in this selection were similar to the criteria listed above, with the following addition:

- Applicability to new technologies developed by Air Products. For the purposes of this
  evaluation, we chose to continue considering all three main elements of the Air Products
  novel technology: Sour PSA, Oxyfuel Combustor, and CO<sub>2</sub> compression with acids
  removal. The costs of producing acids in uncertain quantities and qualities may be a
  remaining issue, and alternate options to consider include:
  - Sulfur Removal:
    - Fuel gas desulfurization (FGD)

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- Wet electrostatic precipitator (WESP) or Membrane WESP for sulfur removal upstream of CO<sub>2</sub> compression and possible Hg removal
- Rectisol® or amine unit to remove H<sub>2</sub>S upstream
- Ammonia scrubbing for SO<sub>2</sub> capture
- Temperature swing adsorption (TSA) to remove SO<sub>3</sub>
- NO<sub>x</sub> removal:
  - Selective catalytic reduction (SCR)
- Haldor-Topsoe SNOX<sup>™</sup> technology for both SO<sub>x</sub> and NO<sub>x</sub> removal

Based upon the ranking by Air Products of the various options, the following were selected for both the hydrogen and power cases utilizing Air Products' technology:

- High-grade heat in the oxy-combustor is used to raise high-pressure steam and to superheat low- and high-pressure steam. Without this provision, the unit generates excess low pressure steam at saturated conditions, which is less valuable in the context of a combined cycle power block.
- A condensing economizer is used on the flue gas from the oxy-combustor to recover energy.
- The dilute acid products would be neutralized and landfilled.
- The use of a cold box to remove inerts was eliminated in favor of achieving the lessstringent CO<sub>2</sub> purity requirements for sequestration instead of EOR.

The resulting flowschemes that were to be compared are as follows:

- Conventional Technology for Hydrogen Production
- Conventional Technology for Power Generation
- Air Products Sour PSA Novel Technology for Hydrogen Production
  - Oxy-combustor superheats LP and HP steam, excess heat used to generate and superheat additional HP steam. Steam used to generate power in steam turbine block.
  - Condensing economizer on oxy-combustor flue gas

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- Dilute acid products neutralized or landfilled
- No cold box; sequestration CO<sub>2</sub> purity requirements
- Air Products Sour PSA Novel Technology for Power Generation
  - Oxy-combustor superheats LP and HP steam, excess heat used to generate and superheat additional HP steam. Steam exported to combined cycle power block.
  - Condensing economizer on oxy-combustor flue gas
  - Dilute acid products neutralized or landfilled
  - No cold box; sequestration CO<sub>2</sub> purity requirements

Note: Alternate options for utilization of the oxy-combustor heat should be considered in future studies, including heating the fuel gas to the gas turbine, pre-heating feed to the gasifier or other industrial applications.

Jacobs Consultancy developed a standard flowscheme for the gasification, gas shift, and cooling sections to maximize heat integration and steam use. This was applied to all four cases so that the upstream portion of each case was the same.

# Appendix A JACOBS Consultancy

### Section 5.



# Case Descriptions & Comparisons

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The basis for the plant design is the target production of approximately 450 MW of net exported power for the power generation base case. This was adjusted to 453 MW to match turbine capacity, resulting in a petcoke feed rate of 4,473 STPD for all four evaluated cases.

This report section compares the results for each of the four flowschemes evaluated, including an overall narrative description of each case configuration, key results data, and a summary of major emissions.

### **Definition of Cases**

As indicated previously, for this study Jacobs Consultancy evaluated four cases:

- Base Case with 4,473 STPD petcoke feed producing 273 MMSCFD H<sub>2</sub>
- Base Case with 4,473 STPD petcoke feed producing 453 MW net power
- Sour PSA Case with 4,473 STPD petcoke feed producing 268 MMSCFD H<sub>2</sub>
- Sour PSA Case with 4,473 STPD petcoke feed producing 473 MW net power

The case configurations are described in detail below. A block flow diagram of the overall process for each of the four cases can be found in Appendix 2. A block flow diagram of the power blocks for the two power cases can be found in Appendix 7. A heat and material balance for the key streams identified in the block flow diagrams for each case can be found in Appendix 3.

### **All Cases**

Coke from storage is mixed with a fluxant and wet-milled to form a coke-water slurry. The petcoke slurry feed is pumped to high pressure, top fired, GE Energy entrained flow gasifiers fitted with a water quench.

The  $O_2$  supplied to the gasifiers is provided by an Air Separation Unit, which generates  $O_2$  at a purity of 99.5% for Hydrogen Cases and 95% for Power Cases. The ASU also supplies  $O_2$  to the Claus sulfur recovery unit in the Conventional Cases and to the Oxy-combustor in the Sour PSA Cases.

In the gasifiers, the petroleum coke slurry is gasified with a sub-stoichiometric amount of  $O_2$  to produce a saturated raw syngas stream consisting primarily of CO and  $H_2$  with some steam,

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CO<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub>, and Ar. The sulfur in the feed is converted primarily to H<sub>2</sub>S with a small amount of COS. Any chlorine in the coke is converted to HCl. Small amounts of HCN and NH<sub>3</sub> are also produced. The inorganic material in the feed is melted in the gasifier and cooled in the quench to form solid slag that is disposed of offsite. The blowdown water is treated and a portion is recycled to the slurry preparation area and the gasifier vessel. Solid waste separated in the waste water treatment plant is disposed of offsite.

Saturated syngas is scrubbed to remove entrained particulates. The scrubber water, together with additional process water, is fed to the gasifier quench chamber as make-up.

The saturated raw syngas stream from the gasifier is passed through a water gas shift reactor section where the CO in the stream reacts with the water vapor in the stream to produce additional H<sub>2</sub> and CO<sub>2</sub>. Heat liberated in this section of the plant is used to raise steam to produce power in a steam turbine (hydrogen cases) or in the combined cycle power block (power cases). The "shifted" syngas stream is then cooled by direct water contact in a desaturator column and the water vapor is condensed and recycled to the gasifier section.

### **Conventional Cases**

The  $H_2S$  in the syngas, together with the bulk of the  $CO_2$ , is then removed in a Rectisol® absorption process. Sour gas from the  $H_2S$  removal process is sent to a Claus sulfur plant. Here, one-third of the  $H_2S$  is combusted to  $SO_2$ , and the gas stream is then passed over a converter where the  $SO_2$  reacts with the remaining  $H_2S$  to form elemental sulfur and water. The elemental sulfur is sold as a by-product from the facility (although no net value was assumed for the sale or disposal of elemental sulfur for the purposes of this study). The tailgas from the Claus unit is hydrogenated, compressed and recycled to the inlet of the Rectisol® unit. Therefore, there are no atmospheric sulfur emissions from the sulfur recovery unit.  $CO_2$  removed from the syngas stream in the Rectisol® unit is compressed to high pressure and is ready for sequestration.

#### **Conventional Power Case**

The sweetened  $H_2$ -rich stream from the Rectisol<sup>®</sup> unit is heated and expanded through an expansion turbine for power generation. It is then mixed with diluent nitrogen (for flame temperature control to limit  $NO_x$  formation), and used as fuel gas in the combined cycle gas turbine power block.

Saturated high pressure and low pressure steam generated by heat recovery elsewhere in the process is also supplied to the CCGT power block.

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### **Conventional Hydrogen Case**

The sweetened syngas leaving the Rectisol<sup>®</sup> unit then passes to a pressure swing adsorption (PSA) unit that generates a high purity H<sub>2</sub> product stream for export. The PSA offgas, which contains CO and unrecovered H<sub>2</sub>, is used as fuel gas in a fired heater to superheat steam raised elsewhere in the process and to generate and superheat additional HP steam.

Superheated high pressure and low pressure steam is supplied in a cascade to the power steam turbine. The power generated by the steam turbine is used internally to offset power demand.

### Air Products' Novel Technology Sour PSA Cases

The cooled, sour "shifted" syngas is passed to a sour pressure swing adsorption (PSA) unit that generates an  $H_2$  product stream and a PSA offgas stream. The PSA offgas—which contains CO, unrecovered  $H_2$ , and  $H_2$ S—is sent to an oxyfuel combustor, where it is mixed with a small amount of natural gas, used as support fuel to increase the calorific value of the stream, and combusted. The heat produced from the combustion is used to superheat steam raised elsewhere in the unit at various pressure levels and to raise and superheat additional HP steam. The combustion products—primarily  $CO_2$  and  $H_2O$ —are further cooled, free water knocked out, compressed to 15 bar, and cooled again. The cooled, compressed gas is passed to a water wash tower where sulfur is removed via conversion of  $SO_2$  to sulfuric acid, and  $NO_x$  is removed via conversion to nitric acid. The process is repeated at 30 bar, with compression, cooling, and water wash to remove the remaining sulfuric and nitric acids. The highly concentrated  $CO_2$  stream is then dried, further compressed to high pressure and is ready for export for sequestration.

### **Sour PSA Power Case**

The  $H_2$ -rich product stream from the PSA is heated and expanded through an expansion turbine for power generation. It is then mixed with diluent gases (for flame temperature control to limit  $NO_x$  formation), and used as fuel gas in the combined cycle gas turbine power block. The diluent gases in this case are  $N_2$ , in the same amount as in the conventional base case, with a small amount of the purified  $CO_2$  stream, compressed to 30 bar, to supplement the  $N_2$  to maintain control of the flame temperature.

Superheated high pressure and low pressure steam generated by heat recovery from the oxyfuel combustor tailgas is also supplied to the CCGT power block.

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### Sour PSA Hydrogen Case

The H<sub>2</sub> product stream from the PSA is exported as high-purity hydrogen product.

Superheated high pressure and low pressure steam generated by heat recovery from the oxyfuel combustor tailgas is supplied in a cascade to the power steam turbine. The power generated by the steam turbine is used internally to offset power demand.

### **Case Comparisons**

The key results for each case are given below in Table 5-1. From a performance standpoint, the Sour PSA cases are nearly identical to the conventional cases. Net power production for the Sour PSA case is more than 4% higher at 473 MW versus 453 MW. Hydrogen production is about the same and is within a few MMSCFD of 270 MMSCFD.

Table 5-1.
Overall Case Results

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Petcoke Consumption (dry)	MTPD	4,472.5	4,472.5	4,472.5	4,472.5
Hydrogen Production	MMSCFD	272.6		268.4	
Power Production/Use					
Power Block Expansion Turbine	MW MW	99	661 7	151 	702 6
Plant Consumption ASU PSA Offgas Compressor CO <sub>2</sub> Compressor Nitrogen Compressor Other Loads Total Consumption Net Power Export	MW MW MW MW MW MW	-91  -54  -38 -183	-89  -47 -42 -38 -215 453	-108 -53 -22  -21 -204 -53	-103 -49 -21 -42 -21 -235 473

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### **Utility Summary**

A summary of major utilities supplied from offsite on a continuous basis is given below in Table 5-2. Although there are differences among the cases, with the exception of power and fuel gas, the cost differences from an operating standpoint are relatively small.

Table 5-2. Utilities Summary

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Electrical Power	MW	83		53	
Natural Gas	MMSCFD			4.3	10.7
Process Water	m³/day	8,517	8,411	8,517	8,135
Steam System Make-Up	m³/day	229	512	366	655
Cooling Water Make-Up	m³/day	52,708	69,829	68,571	83,733
Total Raw Water Required	m³/day	61,454	78,753	77,454	92,523

All other utilities are generated within the plant.

### **Major Emissions and Effluents Summary**

The gaseous, liquid and solid waste streams produced from the gasification plant during normal operation are described below.

#### Gaseous Effluents/Emissions

The major gaseous effluent stream is the flue gas stream from the combined cycle power block in the two power cases and from the fired steam superheater in the conventional hydrogen case. There is no equivalent flue gas stream in the Sour PSA hydrogen case. The expected gaseous emissions from these flue gas streams are listed in Table 5-3. The neutralization of the sulfuric acid with limestone generates CO<sub>2</sub>, which is not sequestered. The amount of CO<sub>2</sub> generated by acid neutralization in the Sour PSA cases is also listed in Table 5-3.

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Table 5-3.

Gaseous Emissions from Power Block / Fired Heater

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Carbon Dioxide (CO <sub>2</sub> )					
Flue Gas Streams	MTPY	230,200	454,338	0	422,184
Acid Neutralization	MTPY			133,064	133,059
Total	MTPY	230,200	454,338	133,064	555,243
Sulfur Dioxide (SO <sub>2</sub> )	MTPY	<1	<1	0	<1
Nitrogen Oxides (NO <sub>x</sub> )	MTPY	20	40	0	30
Carbon Monoxide (CO)	MTPY	101	201	0	186

There are no gaseous emissions from the Claus sulfur recovery unit in the conventional cases, since tail gas is recycled back to the inlet of the Rectisol unit. There are no gaseous emissions from the CO<sub>2</sub> compression & capture section, since the CO<sub>2</sub> product stream will be sequestered and thus is not considered as a source of gaseous emissions. The fraction of the CO<sub>2</sub> product stream that is used as diluent in the power block in the Sour PSA Power Case is included in the Flue Gas Streams' emissions.

Other sources of emissions to atmosphere result from mechanical handling operations in the feedstock storage and preparation areas. Fugitive emissions of process gases from glands, flanges, *etc.* will also be present. As indicated above, the  $CO_2$  emissions for the Hydrogen Sour PSA case are significantly less than the conventional case even when  $CO_2$  capture is present. This is due to the fact that the  $CO_2$  capture is not 100 percent. The  $CO_2$  emissions for the Power Sour PSA case are slightly more than those of the conventional case, with a decreased amount of  $CO_2$  from flue gas streams but an additional  $CO_2$  stream generated by acid neutralization.

### **Liquid Effluent**

The expected liquid effluent streams are listed in Table 5-4.

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Table 5-4. Liquid Effluent

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Gasifier Waste Water	m <sup>3</sup> /h	15	15	15	15
Steam System Blowdown	m³/h	8	18	13	23
Cooling Water System Blowdown	m³/h	1,464	1,940	1,905	2,326
Total Treated Effluent Discharged	m³/h	1,487	1,972	1,933	2,364

#### **Solid Waste Streams**

The only continuous solid waste stream from the plant is process water treating sludge containing the suspended solids and precipitated heavy metals. The sludge may be considered hazardous, depending upon regulations. The flow rates are given below in Table 5-5.

Spent catalysts and water treating resins are assumed to be returned to the catalyst supplier for metals recovery at no cost impact. The value stated in Table 5-5 is an average annual value, as catalysts are typically replaced once every few years.

Coarse slag from the drag conveyor and fine slag in the form of a filter cake from the clarifier are non-hazardous and can be sold as a by-product for road making, construction, and landfill covering. These streams are therefore also excluded from Table 5-5.

Table 5-5. Solid Wastes

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Water Treatment Sludge	MTPD	77	77	77	77
Spent Catalysts and Adsorbents	m³/yr	23	23	23	12

### **Solid By-Product Streams**

Slag is produced as a by-product from gasification in all four cases. Solid sulfur is also produced by the Claus plant in the conventional cases. Wet gypsum is produced as a result of acid neutralization with limestone in the Sour PSA cases. These by-product streams are listed in Table 5-6.

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### Table 5-6. Solid By-Products

Case		Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
Slag	MTPD	224	224	224	224
Solid Sulfur from Claus Plant	MTPD	276	276		
Gypsum	MTPD			1237	1237

# Appendix A JACOBS Consultancy

### Section 6.



# **Capital & Operating Cost Comparisons**

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### **Capital Costs**

### **Basis and Assumptions**

The capital cost estimates for the process areas of the plant were primarily developed by the process unit capacity factoring technique, commonly referred to as cost curves. This technique uses the direct construction costs from previous work and adjusts for capacity as well as other important design differences, time frame and location.

Costs for the utilities and support facilities were estimated as a percentage of the cost of the process units at the direct field cost level based on historical experience.

Costs for certain package units and specialty equipment were obtained from vendors or factored from recent vendor budget quotes and other internal Jacobs data. The ASU cost has been provided by Air Products.

The bases for the capital cost estimates are as follows:

- The capital costs have a ±50% accuracy.
- The costs reflect a 4<sup>th</sup> quarter 2008 time frame.
- Escalation during development and execution of the project is not included.
- Sales taxes are to be included by Air Products.
- Worldwide procurement of equipment and materials has been assumed.
- The costs were developed on a USGC basis, and then converted to an Edmonton, Alberta basis by utilizing an overall capital cost location factor of 1.5 relative to the USGC.
- The capital cost includes the following major areas in the plant, as appropriate to each case:
  - Feedstock receiving, storage, primary crushing, and handling
  - Air separation unit
  - Feed preparation
  - Gasification, including carbon scrubbing, fines handling and slag handling
  - Gas cooling and shift unit

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- Acid gas removal
- Sulfur plant
- Conventional PSA hydrogen purification
- Sour PSA hydrogen purification
- Sour PSA tailgas oxy-combustion
- Oxy-combustion tail gas compression
- Sulfuric/nitric acid recovery & neutralization
- CO<sub>2</sub> dehydration & compression
- Power generation
- Utilities and support facilities for a greenfield plant:
  - Raw water treating
  - Electrical distribution
  - Communications system
  - UPS system
  - Waste water treating
  - Steam & condensate distribution
  - Fire water
  - Plant control and management information system
  - Site preparation
  - Roads, paving, fencing, lighting
  - Buildings
  - Cooling tower/cooling water
  - Potable/utility water
  - Sanitary waste treatment
  - Demineralization

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- Plant & instrument air
- Flare
- Sewers
- Nitrogen system
- Fuel gas system
- Interconnecting piping between units
- Connections to the surrounding infrastructure as listed below are excluded:
  - Interconnecting piping between the gasification plant and the users of the hydrogen product
  - Facilities for supply of electric power, raw water and natural gas
  - Facilities for the export of electric power
  - Facilities for long-term disposal of solid wastes
  - Pipelines for export of CO<sub>2</sub> to sequestration facility
  - Pipelines for disposal of liquid wastes

The gasification unit includes a spare gasifier train in the hydrogen cases only.

The estimated capital cost includes the following components:

- Field costs
  - Direct field material
    - Equipment
    - Bulk materials (concrete, piping, electrical cable, instruments, etc.)
  - Direct field labor
  - Indirect costs
- Construction management
- Home office costs

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- Project management contractor costs
- Contingency

A contingency of 20% has been included based on historical experience for similar projects in this early stage of development.

The cost represents the EPC cost of the project because it includes the typical scope of the EPC contractor. Owner's costs are discussed further below.

### **Capital Cost Summary**

The capital cost for the plant is given in Table 6-1 below. The table includes a breakdown of the costs into the major areas of the plant and major costs elements.

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Table 6-1. Capital Cost Breakdown

Case	Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
	\$ million	\$ million	\$ million	\$ million
Air Separation Unit	316.7	307.1	343.0	330.9
Petcoke Receiving, Storage & Handling	19.0	19.0	19.1	19.1
Gasification Including Feed Preparation	286.1	237.0	286.1	237.0
Gas Cooling and Shift Conversion	273.0	275.0	273.0	233.7
Acid Gas Removal*	286.3	288.4		
Sulfur Recovery	122.7	122.7		
Hydrogen Purification	49.0			
Sour PSA			154.4	115.0
Sour Gas Oxy-Combustion			108.3	98.4
Flue Gas Compression & Acid Recovery			146.6	146.6
CO <sub>2</sub> Drying & Compression	60.6	58.4	15.5	14.8
Power Block	45.3	418.6	61.3	453.1
Utilities & Support Facilities	366.8	431.6	349.4	409.9
Field Costs	1,825.5	2,157.8	1,756.5	2,058.5
Home Office Costs	275.1	323.7	263.5	308.8
Construction Management Costs	55.0	64.7	52.7	61.8
Overall Project Management Contractor Costs	108.2	127.3	103.6	121.4
Total before Contingency	2,263.8	2,673.5	2,176.2	2,550.4
Contingency	454.5	534.7	435.2	510.1
Project Total Installed Cost	2,718	3,208	2,612	3,061

\*Note: Air Products also has experience with Rectisol units, and there were slight differences between the estimated capital costs for the Rectisol system. For consistency, Jacobs Consultancy's estimated capital cost was used; differences may occur with regard to efficiency of refrigeration and alternate regeneration methods, among other reasons.

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### **Owner's Costs**

### **Basis and Assumptions**

The above TIC represents the EPC cost of the project. Owner's costs that can be outside of the scope of the EPC contractor are listed below and discussed in this section:

- Initial catalysts and chemicals
- Spare parts
- Commissioning and start-up
- Land
- Permitting
- · Furniture, laboratory equipment, mobile equipment
- Owner's project management
- Project development—studies, legal and financial consultants
- Operator training
- Insurance during construction
- Process technology license fees
- Interest during construction
- Financing fees
- Working capital
- Escalation

Of the above costs, the following costs are generally considered as part of the financial analysis, and are dependent upon the financing mechanism and assumptions made in the analysis:

- Interest during construction
- Financing fees
- Working capital
- Escalation

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A brief discussion of the basis for allowances of the other Owner's costs is given below. The costs are based on previous project experience and guidelines of EPRI, IEA and other organizations. For the more difficult-to-estimate costs that can vary widely among projects, rough allowances have been included. The accuracy of these costs can be considered to be less than that of the plant capital cost.

### **Initial Catalysts and Chemicals**

These items include the initial charge of catalysts and chemicals required to make the plant fully operational. The initial fill costs are based on factored estimates from similar projects.

### **Spare Parts Inventory**

The cost of spare parts inventory is estimated to be 2% of the plant Field Cost.

### **Commissioning and Start-Up**

Commissioning and start-up costs cover testing of the individual items of equipment and systems in the plant followed by starting up of the plant and resolving operational issues until the plant is capable of passing a performance test. It includes the cost of contractor, licensor and vendor representatives for this activity. It is estimated as 2% of the plant Field Cost.

### Land

The cost of land can be highly variable depending upon the location. An allowance of \$2 million has been included. Air Products can adjust this based on discussions regarding a specific site.

### **Environmental Permitting**

An allowance of \$5 million has been included for the costs related to environmental permitting such as site investigations, engineering studies, and preparation of environmental permit applications. This cost can vary widely among locations depending upon the environmental sensitivity of the particular site and local regulations. Air Products can adjust this cost based on discussions with its environmental consultant.

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# Plant Mobile Equipment / Furniture / Lab and Shop Equipment

An allowance of \$1 million has been included for the costs of plant mobile equipment (trucks, maintenance equipment, etc.), office furniture, laboratory equipment and maintenance shop equipment.

### **Owner's Project Management**

An allowance of \$7 million has been included for the costs associated with Owner's representatives providing guidance to the overall project management contractor and the contractors that design and build the project

### **Project Development**

This category includes costs for various project development activities such as feasibility studies; development of contracts for feedstock, products, construction, operation, *etc.*; negotiation of licensing agreements; and development of financing arrangements. These are primarily business-related activities required to bring the project to the point of financial close. A FEED package is not included in this cost because it is part of the EPC cost. An allowance of \$5 million has been included to cover these costs.

### **Operator Training**

A key group of operators will require both classroom training and training at a similar plant. An allowance of \$3 million is provided for this cost.

### **Insurance**

An allowance of 1% of the TIC is considered for the insurance costs for the project.

### **Process Technology License Fees**

An allowance of \$30 million is considered for the technology license fees for the various process technologies used for the project. These licensor fees need to be confirmed after final selection of the technologies to be utilized.

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### **Owner's Cost Summary**

Owner's costs are summarized in Table 6-2.

Table 6-2. Owner's Cost Summary

Case	Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
	\$ million	\$ million	\$ million	\$ million
Initial Catalysts & Chemicals	10	10	10	10
Spare Parts Inventory	37	43	36	42
Commissioning & Start-up	37	43	36	42
Land	2	2	2	2
Environmental Permitting	5	5	5	5
Plant Mobile Equipment/ Furniture/ Laboratory & Shop Equipment	1	1	1	1
Owner's Project Management	7	7	7	7
Project Development	5	5	5	5
Operator Training	3	3	3	3
Insurance	27	32	26	31
Process Technology License Fees	30	30	30	30
Total	164	181	161	178

### **Operating & Maintenance Costs**

Operating and maintenance costs, excluding the feedstock, are divided into fixed and variable components. Fixed costs are independent of the plant operating factor and include the following items:

- Operating labor
- General & administrative
- Maintenance
- Property taxes
- Insurance

Variable costs are dependent on the plant operating factor and include the following items:

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- Utilities
- Catalysts & chemicals
- Waste disposal
- Slag (credit)

The catalyst was assumed to have an absorbent life of 15 years.

For preliminary evaluations, annual operating and maintenance costs—exclusive of feedstock, power, sulfur disposal and acid neutralization Costs—can be estimated as approximately 5% of the TIC of the plant (represented as "Other O&M Costs" in Table 6-3). Additionally, the costs of imported power and natural gas, the shipping cost for sulfur disposal in the conventional cases, and the limestone and gypsum shipping costs for acid neutralization in the sour PSA cases are included in Table 6-3.

Table 6-3.
Operating & Maintenance Cost Summary

Case	Conventional Hydrogen	Conventional Power	Sour PSA Hydrogen	Sour PSA Power
	\$ million/yr	\$ million/yr	\$ million/yr	\$ million/yr
Net Imported Power	60		38	
Natural Gas			14	30
Sulfur Disposal	1	1		
Acid Neutralization Costs:				
Limestone			30	30
Gypsum Shipping			6	6
Other O&M Costs	136	160	131	153
Annual O&M Costs	197	162	218	218

## Appendix A JACOBS Consultancy

### Section 7.



### Semi-Quantitative Technology Risk Analysis & HAZID Review

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### **Semi-QTRA**

On January 15, 2009, Jacobs Consultancy facilitated a semi-quantitative technology development risk analysis session with Air Products, covering its new Advanced CO<sub>2</sub> Capture Technology for Gasification.

The objective of this exercise was to:

- Identify potential technology performance and technology cost issues that might cause the technology not to meet the expected performance or to exceed estimated capital and operating costs.
- 2. Identify any potential fatal flaws related to technology development and operation.
- 3. Estimate the most important (key) potential Risk Issues and then estimate the probability of occurrence for each Risk Issue as well as the potential value of the risk event.
- 4. Use this semi-quantitative analysis to decide which risks need attention in terms of (a) design-arounds or other mitigation activities and (b) additional analysis.
- 5. Determine the need for a more quantitative version of risk analysis.

The session did not focus on HS&E issues since these were covered in a separate HAZID exercise.

### **Part 1: Initial Risk Identification**

For the Primary PSA Design Case, thirty-nine individual Risk Issues were identified by the Air Products process development project Team with the assistance of Jacobs Consultancy's process development consultants. These Risk Issues are summarized in Table 7-1.

An initial triage step was performed on these thirty-nine potential Risk Issues, and fourteen Risk Issues were selected as having a potential degree of impact value and probability that warranted further (semi-quantitative) analysis. These Top 14 issues are denoted in Table 7-1 by underlined Risk Numbers.

The basis for this analysis was a plant that was fully commissioned and ready to run at operating conditions.

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### Part 2: Initial Risk Semi-Quantification

The fourteen Top Risk Issues were taken through a semi-quantitative risk analysis process that bracketed (a) potential risk impact on the ultimate project value and (2) the probability of impact occurrence.

To bracket the potential risk event value and event probability of occurrence, a modified (opensession) Delphi-method was used to develop estimated ranges of event value and event probability from the Air Products process development Project Team. The results of this facilitated risk quantifying session are summarized in the Project Risk Register, which will be attached to this report as a digital MSExcel file. The key sections of the Project Risk Register are included in Appendix 4.

The Risk Issue values were typically of four types:

- 1. Additional Capex for a typical technology installation
- 2. Temporary or permanent additional Opex for a typical technology installation
- 3. Temporary or permanent loss of operating margin for a typical technology installation
- 4. Shift of project design, construction and start-up time into the future.

Each of these Risk Issue values was inserted into a simple NPV model of the project, and a delta project NPV was calculated for each Risk Issue. The delta NPV is an estimate of the project value loss that a new technology user would suffer if the risk event occurred.

[A simple 20-year delta NPV model was used to calculate delta NPV. A discount rate of 12% was used. Terminal value was not calculated. The delta NPV models used to calculate each risk's potential impact value are included in the Risk Register.]

Thus, for each of the top fourteen Risk Issues, we arrived at a key pair of values, a most likely delta project NPV and a most likely probability of Risk Issue (or event) occurrence. These values are shown, for each of the top fourteen Risk Issues, in Table 7-2.

Also shown in Table 7-2, as applicable, are the ranges of delta NPV and event probability when ranges were estimated as part of the risk quantification process. Extraordinarily high risk values and high risk probabilities are highlighted in Table 7-2.

[This risk-bracketing process is called semi-quantitative due to its approximate and subjective nature. It is not a substitute for a more rigorous quantitative risk analysis, which is always

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recommended for capital intensive process development projects. In addition, it is possible that some of the potential risks from the list of thirty-nine that did not make the "Top Fourteen" cut will indeed turn out to be critical risk issues, as process development continues and more knowledge about probable process performance is gathered. The entire list of 39 risk issues should be revisited and reconsidered regularly.]

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Table 7-1. Primary Case Risks Identified

Risk No.	Potential Risk (Uncertainty) Issues
<u>1</u>	PSA Adsorbent dies faster than originally planned changeout schedule (10 year basis)
2	PSA recovery is lower than predicted
3	Sulfuric acid is not saleable
4	More aggressive than planned corrosion in vessels (particularly reaction system and
5	Excessive heat within combustor and all tail gas cannot be processed
<u>6</u>	Variability in feedstock composition beyond expectations
7	Downtime is greater than expected due to failures
<u>8</u>	Mechanical issues caused by corrosion in PSA
9	Mercury or metals in higher levels than anticipated in acid streams via PSA off gas
<u>10</u>	Excessive capital requirements for acid section
11	Acid-based corrosion in combustor and heat exchangers
<u>12</u>	More support fuel required in oxy-combuster than originally expected
<u>13</u>	Acid reactions do not occur as predicted; incomplete conversion of SO2 into sulfuric acid
14	Air ingress to combustor
<u>15</u>	CO2 spec is not met
<u>16</u>	CO2 Regulatory specs end up to be tighter than design basis specs. [Assume this is a spec in place that is changed.]
<u>17</u>	Extra downtime due to solving problems with heavy metals
18	Higher pressure PSA operation affects mechanical integrity
19	Unexpected acid condensation resulting in corrosion, control problems, downtime
20	Price collapse for CO2
21	Price collapse for acid
22	Price collapse for power (can go to H2)
23	Capex increase
24	Additional Capex from not meeting CO2
25	Inability to meet H2 pipeline spec with PSA
26	Compressor reliability
27	Water availability
28	Possible need for zero liquid discharge
29	Total Installed Cost is greater than plans
30	Downtime or initial capex from replacing failed compressors
31	Downtime or capex resulting from combustor replacement/repair issues
32	Takes more than 12 months to reach design operation
33	CO2 may not be able to be vented if pipeline is unavailable
<u>34</u>	Development time extended due to change in feedstock
35	Increased power requirements of compressors
36	Plant complexity requires additional operators
37	Exceed sulfur emissions quota
38	Design & construction & procurement schedule delays
<u>39</u>	Long-term liability cost due to land spread of H2SO4

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Figure 7-1 is a representation of the top 13 Risk Issues on a Risk versus Probability Grid. (The Top 14 risks were ultimately shortened to 13 because Risk 8 was covered by the treatment of Risk 4.) This graphic is a simple way to picture the relative values and probabilities of each risk and see if any value X probability combination leads to a potential risk-adjusted value that would present an immediate issue to the project.

The most likely risk event values and risk occurrence probability values, for all 13 Top Risk Issues, are pictured by the 13 smaller symbols. The rose-colored boxes around each symbol represent the range of probability and value estimated for each risk issue, as applicable. Risk issues surrounded by large rose colored boxes have a lot of uncertainty related to value and probability.

Any project with a combination of high value and high probability is an obvious concern.

Without knowing the estimated NPV for this project, it is not possible to know if any of the values depicted on Figure 7-1 and Table 7-2 are of significant concern in terms of having a significant effect on project viability. Typically, when one knows the expected and minimum acceptable NPV of a project, the corresponding minimum delta NPV value can be noted on this type of grid and guide relative ranking of risk and investment in efforts directed at risk mitigation. In general, values in the upper left hand quadrant are often critical risk issues.

In this semi-quantitative analysis, Risk Issues 3, 4, 15 and 17 are the most potentially critical, on a relative basis. Criticality is judged not only by proximity of average values, but also by the range of probable values.

In summary the most critical Risks Issues we identified are:

- RISK 3: Sulfuric acid is not saleable. [This risk issue is no longer pertinent to this technology application, as Jacobs Consultancy's market analysis has shown that there is not enough of a market for low concentration sulfuric acid in the Western Canada region. We are keeping the risk analysis in the risk register, regardless, as a record of the analysis. It could prove useful for applications of this technology in different geographic locations.]
- RISK 4: More aggressive than planned corrosion in vessels, particularly reaction system and piping. [This is an item that Jacobs Consultancy often sees as a top Risk Issue. In fact, Jacobs Consultancy often sees the recognition of potential risks related to corrosion issue effects increase as process development projects progress and as design and process development engineers learn more about potential process chemistry and surface chemistry issues.]

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- RISK 15: CO<sub>2</sub> specifications not met
- RISK 17: Extra downtime due to solving problems with heavy metals

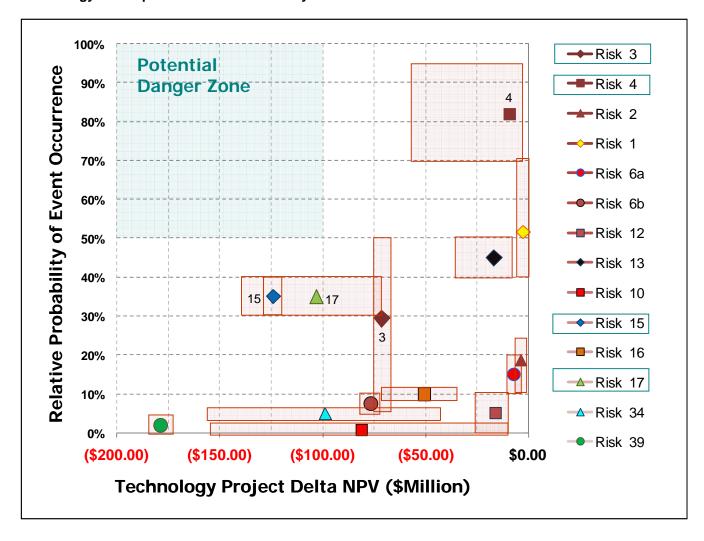


Table 7-2. Primary Case Key Risk Issues

Risk	Risk Description	Most Likely Impact Value (\$MM delta NPV)	Most Likely Impact Probability	_	ilue Range elta NPV)	Probability Range		
		NFV)		Low	High	Low	High	
Risk 3	Sulfuric acid is not saleable	(\$71.5)	29%	na	na	5%	50%	
Risk 4	More aggressive than planned corrosion in vessels (particularly reaction system and piping)	(\$9.5)	82%	(\$0.9)	(\$67.0)	70%	95%	
Risk 2	PSA recovery (R) is lower than predicted	(\$3.9)	19%	na	na	10%	25%	
Risk 1	PSA Adsorbent dies faster than originally planned changeout schedule (10 year basis)	(\$2.7)	52%	(\$1.4)	(\$4.6)	40%	70%	
Risk 6a	Variability in feedstock composition beyond expectations	(\$7.7)	15%	na	na	10%	20%	
Risk 6b	Variability in feedstock composition beyond expectations	(\$76.6)	8%	na	na	5%	10%	
Risk 8	Mechanical issues caused by corrosion in PSA	covered as p	art of Risk 4	na	na	na	na	
Risk 12	More support fuel required in oxycombustor	(\$16.3)	5%	(\$12.2)	(\$24.5)	1%	10%	
Risk 13	Acid reactions do not occur as predicted, incomplete conversion of SO2 into sulfuric acid	(\$17.0)	45%	(\$6.8)	(\$34.1)	40%	50%	
Risk 10	Excessive capital requirements for acid section	(\$81.4)	1%	(\$7.1)	(\$155.7)	0.5%	1.0%	
Risk 15	CO2 spec is not met	(\$123.9)	35%	na	na	30%	40%	
Risk 16	CO2 Regulatory specs end up to be tighter than design (expectation) [Assume this is a spec in place that is changed.]	(\$50.7)	10%	(\$32.5)	(\$68.9)	na	na	
Risk 17	Extra downtime due to solving problems with heavy metals	(\$103.1)	35%	(\$68.8)	(\$137.5)	30%	40%	
Risk 34	Development time extended due to change in feedstock	(\$98.8)	5%	(\$39.4)	(\$158.2)	na	na	
Risk 39	Long-term liability cost due to landspread	(\$178.6)	2%	na	na	na	na	

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Figure 7-1.
Technology Development Risk vs. Probability Grid for Base Case



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All 13 Top Risk Issues deserve further attention, but Risk Issues 3, 4, 15 and 17 should be reviewed immediately and be the top priority, in terms of potential risk mitigation process development plans.

### Risk Issue Adjustments for Configuration Cases "B" and "C"

The alternate configuration cases "B" and "C" were evaluated in terms of how their implementation might change the semi-quantitative risk analysis.

- Case B: Additional heat recovery in / after oxy-combustor
- Case C: Acids neutralized and landfilled

This was a completely qualitative analysis. The intent is to give Air Products high-level guidance related to potential increase or decrease in project risk—relative to the Primary Case—for the two process configuration options.

A summary of the potential deviations from the Primary Case risk analysis, for Configuration cases B and C, is shown as Table 7-3.

#### **General Recommendations**

- A Semi-Quantitative Risk analysis should be performed on all the elements of Case B
  that differentiate it from the Primary Case. (Case B now appears to be the "operative"
  flowscheme for the new technology.) The qualitative risk analysis for Case B shows
  some potentially key differential risks.
- Re-evaluate Risk Issues 4, 15 and 17.
- Once pilot plant work is complete, conduct a full project Quantitative Risk Analysis (QRA), covering the following issues:
  - Capital expenditure estimates (Capex)
  - Opex estimates (labor, maintenance, insurance, disposal costs, etc.)
  - Sustaining Capex
  - Construction time estimates (schedule risk)
  - Feedstock prices, other raw material prices, and product values

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- Logistics risk
- Currency risk
- Product demand growth rates
- Competitive response
- Finance rates, Inflation rates
- Taxes, tariffs, logistics constraints
- Technology performance and unit availability
- Regulatory, HS&E Risk
- Political risk



Table 7-3.

Qualitative Risk Analysis of Alternative Configuration Cases A and B, versus Primary Case

Risk	Risk Description	Most Likely Impact Value (\$MM delta NPV)	Most Likely Impact Probability	Alternate Configuration Case "B - Additional heat recovery in / after oxy-combustor" [Probable Deviations from Base Case Risk Analysis]	Alternate Configuration Case "C - Neutralization" [Probable Deviations from Base Case Risk Analysis]
Risk 3	Sulfuric acid is not saleable	(\$71.5)	29%	No significant change	Sales becomes non issue. However will now need to worry about full disposal cost and multiple exposure issue risks.
Risk 4	More aggressive than planned corrosion in vessels (particularly reaction system and piping)	(\$9.5)	82%	Risk impact is same, generally, but Probability increases slightly	no significant change
Risk 2	PSA recovery (R) is lower than predicted	(\$3.9)	19%	no significant change	no significant change
Risk 1	PSA Adsorbent dies faster than originally planned changeout schedule (10 year basis)	(\$2.7)	52%	no significant change	no significant change
Risk 6a	Variability in feedstock composition beyond expectations	(\$7.7)	15%	no significant change	More S means more neutralization.
Risk 6b	Variability in feedstock composition beyond expectations	(\$76.6)	8%	Could reduce impact.	no significant change
Risk 8	Mechanical issues caused by corrosion in PSA	covered as p	art of Risk 4	na	na
Risk 12	More support fuel required in oxycombustor	(\$16.3)	5%	no significant change	no significant change
Risk 13	Acid reactions do not occur as predicted, incomplete conversion of SO2 into sulfuric acid	(\$17.0)	45%	no significant change	less to neutralize
Risk 10	Excessive capital requirements for acid section	(\$81.4)	1%	no significant change	no significant change
Risk 15	CO2 spec is not met	(\$123.9)	35%	no significant change	no significant change
Risk 16	CO2 Regulatory specs end up to be tighter than design (expectation) [Assume this is a spec in place that is	(\$50.7)	10%	no significant change	no significant change
Risk 17	Extra downtime due to solving problems with heavy metals	(\$103.1)	35%	Slight increase in probability	Might cost more to dispose or landfill. Might increase risk of post- spread exposure issues.
Risk 34	Development time extended due to change in feedstock	(\$98.8)	5%	no significant change	no significant change
Risk 39	Long-term liability cost due to landspread	(\$178.6)	2%	no significant change	no significant change

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#### **HAZID**

On January 14<sup>th</sup> and 15<sup>th</sup>, 2009, Jacobs Consultancy facilitated a HAZID-Lite (High level Hazards Identification process performed at process concept stage) session for the Air Products Advanced CO<sub>2</sub> Capture Technology for Gasification process.

This was not a formal HAZID session, as the Air Products process design is still in the conceptual stage. Rather, this was a high-level analysis, designed to capture basic HAZOP (Hazard and Operability Analysis) issues. Other common names for this level of exercise are PrHA (Preliminary Hazards Analysis) and SLRA (Screening Level Risk Analysis).

The objective of this 1.5-day exercise was to:

- 1. Identify and construct a list of potential hazards and hazardous situations related to the new process technology operation.
- Identify issues requiring attention during the development and design phase of the project. (Guide final configuration development, design basis formulation and preliminary design.)
- 3. Screen the Base Case (primary Sour PSA flowscheme) and 2 top alternative process flowschemes, to facilitate selection of top flowscheme for further analysis.
- 4. Identify potential "Fatal Flaws."
- 5. Record all issues in a HAZID-Register that can be used as the basis for HAZOP-issue capture and response accounting.

### **Step 1: Setting Basis of Analysis**

The participants were instructed to consider the "ready to operate" plant. They were told to consider start-up, ongoing operations, and shutdown (or hold) phases of operation. They were told to assume that the typical levels of instrumentation, tankage, control systems and offsites would be in place.

The working definition of HAZARD the participants were instructed to use was:

A potential event or activity (action) that could possibly cause or result in:

Release of flammable, explosive or toxic materials

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- Injury to personnel or harm to the environment
- Major loss of asset value or operating revenue.

The participants were instructed not to consider technology performance risk, as that would be covered in a separate risk analysis session.

### Step 2: Developing a List of Potentially Critical Substances

The session participants were asked to brainstorm to develop a list all substances that would likely be used, created or stored in the process environment. These were defined as Potentially Critical Substances.

This brainstorming was conducted by evaluating sequential process streams. The List of Potentially Critical Substances developed is shown in Hazard and Operability Analysis Table 7-4 and Table 7-5.

### **Step 3: High-Level HAZID on Primary Case Flowscheme**

In this final step the session participants were asked to brainstorm and consider the possibility of internal and external actions and events, involving the identified critical substances that might immediately or ultimately lead to any of the following events in the proposed process flowscheme:

- toxic exposure or injury
- fire
- explosion
- corrosion or erosion

The potential hazards identified are located in the HAZID register, which is reproduced in Appendix 5.

### Step 4: High Level HAZID on Two Alternate Flowschemes

This session was facilitated in the same manner as the session on the basic flowscheme.

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The potential hazards identified are located in the HAZID register, which is reproduced in Appendix 6.



Table 7-4. List of Critical Materials Part 1

List of Potentially (	Critical Substances: Part 1										
Stream Name (or Location )	Potential Critical Material in Stream [and key notes related to critical materials or their reaction or capture, etc.]										
SynGas	H2, CO, CO2, H2S, COS, N2, Ar, CI compounds CI <sub>n</sub> -X (HCI), residual Hg (at times), Hg at low levels always, Arsenic, Metal-Carbonyls, CH4, NH3 (trace), CN-, H2O, CS2										
Not expected: Vanadium/Nickel (go to slag), HF (may be present in co F in petcoke)											
Natural Gas (support fuel to combustor)	CH4 and also C2, C3, C4, odorant compounds (mercaptans)										
High-Purity Oxygen	O2 (99.5% for H2 case, balance is Ar; 95% for Power case, 3% Ar and 2% N2)										
Out of PSA	Nothing coming off of adsorbent (Zeolites, Carbons, aluminas Al2O3, silica gels SiO2). Standard size/shape separation. No issues of anything being chemically displaced. Potential for dust coming out of PSA on initial cycles. [Perhaps we can use a filter? Waste disposal of spent adsorbent will be discussed later.]										
Outlet of combustor	NOx (NO2, NO, N2O unlikely), SOx (SO2, SO3 trace), CO (trace), CO2, H2O, Ar, N2, O2 (trace), soot (carbon particles), refractory components (Silica), also trace amounts of syngas feed components and oxidized versions (H2S, metal oxides, Cl-oxides, Hg species), Hg + Cl = ? [May react in the gasifier? Would Hg removal also remove Hg-Cl compounds? Paul Cottrell says Hg removal processes (activated charcoal impregnated with sulfur) will remove it. Look into acid resin capture.]										
Flue gas cooler/condenser	H2O + outlet of combustor, H2SO4, carbonic acid, HNO3 (trace), H2O + Cl-X = ? (Chlorine will react with water, also with Hg probably in combustor). [We need to find out what happens with H2O and Cl. Need to understand as function of temperature, as function of concentration. This will vary with feedstock type. May require a treater (catch-all treater with arsenic.]										



Table 7-5. List of Critical Materials Part 2

List of Potentially	Critical Substances: Part 2
Stream Name (or Location )	Potential Critical Material in Stream [and key notes related to critical materials or their reaction or capture, etc.]
In/Out of Acid formation & separation	H2O, H2SO4, HNO3, Hg-oxides, Hg-nitrates, dissolved gases. [Liquid streams will have dissolved CO2, N2, Ar, O2 at 15 and 30 bar]
Dehydration Step	Product: CO2, N2, O2, Ar, dust from TSA beds. Regen Gas: H2O, residual H2SO4, HNO3, SO3, NO2, SO2, dust from TSA beds, Regen Gas TBD (N2, ?). [Downstream filters? If we have a coldbox, we would add a guard bed before the cold box.]
Cold Box	CO2, N2, O2, Ar. Vent: CO2 (trace), CO, O2, Ar, + what comes through from feed.
Compression	CO2, N2, O2, Ar (Supercritical). [We may get 2 phases if we have too many noncondensables with 95% purity. May be a risk if we are sending 2 phases to a pump.]
H2 to power block	Power scheme: H2 to expander, to preheater, to gas turbine combustor (with addition of N2 & air for combustion). Combustion products to HRSG, to potential SCR, to stack. Same as conventional equipment. Inlet gas is H2, CO, CH4, CO2, H2S (trace), N2 (trace), Ar (trace), no Hg, Dust, Metalcarbonyls, H2O (trace), COS (trace). [If we haven't adequately preheated before the expander, could get liquid water etc. or ice. No change across preheater.]
Power Turbine Combustor Out	Inlet + NOx, SO2, SO3, O2, N2, H2O, CO2, soot
SCR	In: NH3. Out: excess NH3, NH4SOx, SO2>SO3
H2 Production Case	H2 product at pressure. No change
Steam System	?? [Power case: BFW in from supply. Use power block BFW treatment. Steam, BFW, Blowdown out. HRSG uses flue gas out of turbine to raise steam] [novel flue gas on HX surfaces.]
Steam Gen at Oxycombustor	?? [Novel flue gas on HX surfaces to raise/superheat steam.]
Used Adsorbent "Stream"	H2S, CO, possible heavy metals (depending on feed), carbonyls. Hazardous waste?
Misc Knock-Out Liquids	None identified.

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#### **Recommendations and Final Notes**

- 1. Review MSDS for all Potential Critical Substances.
- 2. Review all HAZOP items in more detail after target process flowscheme is selected.
- 3. Perform a HAZOP ranking session to determine high-probability major design-arounds that should be incorporated into the process design. (These should become part of the next cost estimate.)
- 4. Refer to the Jacobs Consultancy January 14 -15 Meeting Notes for a more detailed summary of the HAZID-Lite session.

# Appendix A JACOBS Consultancy

# Section 8.



# **Summary & Recommendations**

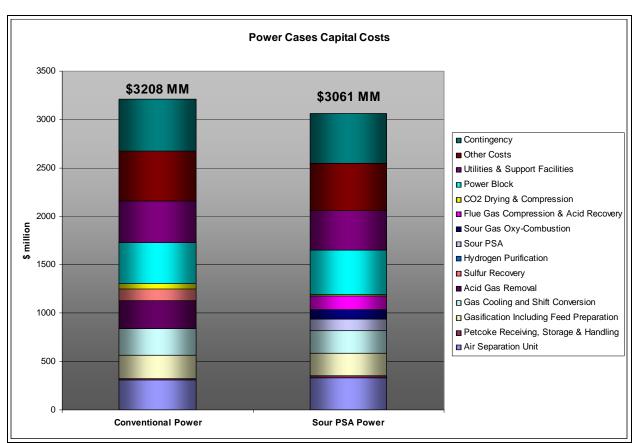
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Air Products' Sour PSA technology has the potential to reduce capital costs and incrementally improve CO<sub>2</sub> recovery when compared to Conventional Gasification technology in a commercially sized application. The focus, however, for technology development should be aimed not only at ensuring performance advantages but also at reducing capital costs further and developing alternate and less expensive options for removing sulfur—and, to a smaller extent, nitrogen components—from the PSA offgas.

# **Capital Costs**

Based on our review of the capital costs, the Sour PSA technology has the potential to reduce capital costs for both the hydrogen and power case on a standalone basis by \$110 to \$150 MM on a total investment of around \$2,600 to 3,100 MM. Although the savings are well within the accuracy intervals of the estimates (±50%), we can compare the mid-point costs for each case. Figures 8-1 and 8-2 below summarize the mid-point costs for each case.



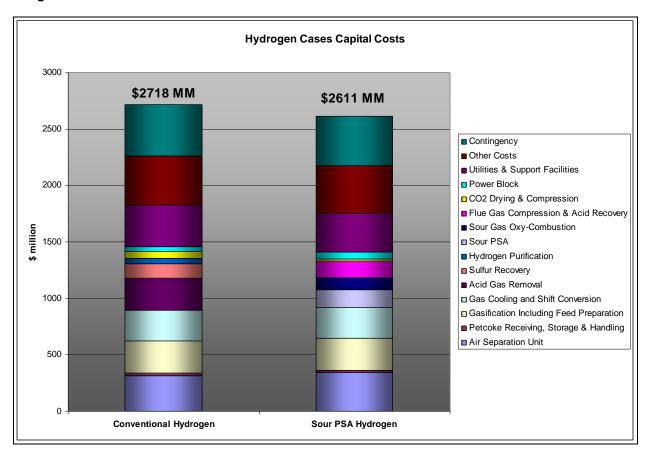


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# Appendix A JACOBS Consultancy

The savings for the Sour PSA in the power case is about \$150 MM.

Figure 8-2.



Note: The Acid Gas removal costs include compression up to 30 bar for the Sour PSA cases.

The capital cost savings for the Hydrogen case are smaller than the power at roughly \$110 MM. This is primarily due to the more expensive Sour PSA equipment required for the Hydrogen Case. However, it should be noted that the savings we show for the Sour PSA cases represent only about 4 to 5% of the total costs and are well within the noise of the estimates, which is ±50 percent. While the range of uncertainty in the actual costs should be the same for each case, the actual costs for constructing new technology are often skewed toward the high side of original estimates.

Furthermore, the savings could be much less for gasification plants that are situated near upgraders or refineries. In these situations, incremental investment in existing sulfur units would be substantially cheaper than a dedicated sulfur plant for a gasification block, and would therefore reduce the capital costs for the conventional technology. For these reasons, we opine

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that an important aspect of the technology development program should be aimed at further reducing the capital costs.

Key drivers for the capex reduction in both the Hydrogen and Power Sour PSA Cases vs. the Conventional Cases are as follows:

- Elimination of the entire Rectisol unit
- Elimination of the Sulfur Recovery unit
- Other factored expenses and contingency

Despite the elimination of these components, there are important cost considerations for the Sour PSA technology, including:

- Sour PSA system
- Sour Oxy-Combustor plus a larger ASU to provide high-purity oxygen
- Compressor equipment in the acid removal section requiring enhanced metallurgy

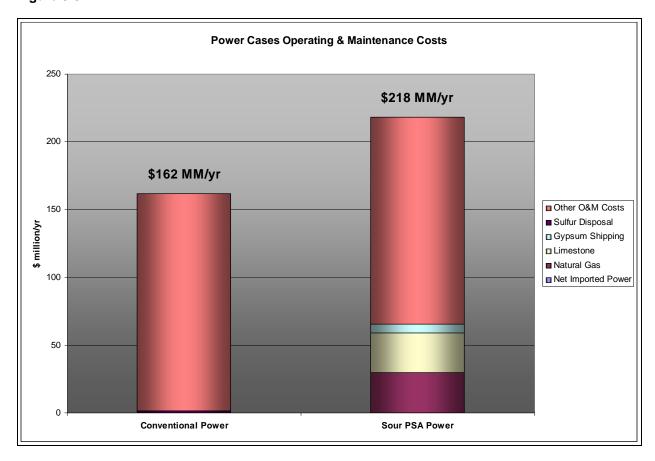
## **Operating Expenses**

Based on our estimates of the operating expenses, the Sour PSA technology appears to have higher operating expenses primarily due to the acid neutralization costs. In addition to capital cost considerations, alternatives for the disposition of the sulfur-related compounds should be considered. The sulfuric acid production is anticipated to be relatively dilute and contaminated with some nitric acid. In addition, even in a pure state, the sulfuric acid volume is large relative to the market size.

Our preliminary market analysis indicates that the sulfuric acid production from this single preliminary design would be enough to supply the whole Western Canada market, and represents nearly 1% of the total North American market. Therefore, we expect that the acid would have to be neutralized and the resulting gypsum landfilled. Total costs for this are expected to be \$33,000,000 - \$40,000,000 per year, putting the Sour PSA at a distinct operating cost disadvantage relative to conventional technology, which produces about 100,000 MT/yr of sulfur that, if not sold, can be readily stored safely and indefinitely. Figures 8-3 and 8-4 below summarize the operating costs for the Power and Hydrogen cases.

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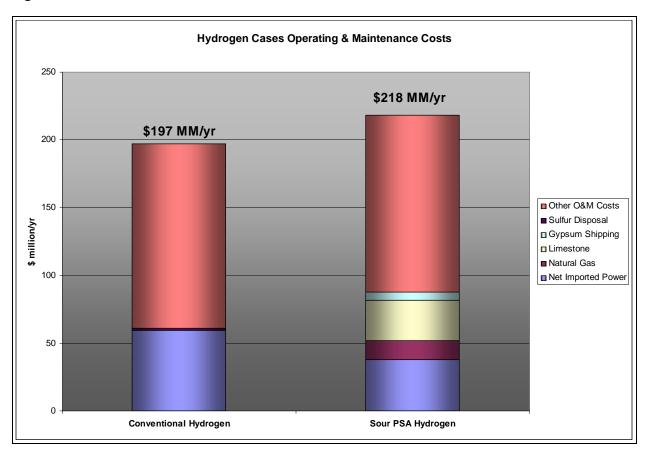
Figure 8-3.



In the Power case comparison, the operating costs for the Sour PSA case are roughly \$60 MM/yr higher due primarily to the neutralization costs as well as the incremental natural gas required for the Sour Oxy-Combustor.

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Figure 8-4.



In the Hydrogen case comparison, the operating costs for the Sour PSA case are only about \$20 MM higher with the neutralization costs offset by a reduction in the power required.

## CO<sub>2</sub> Recovery

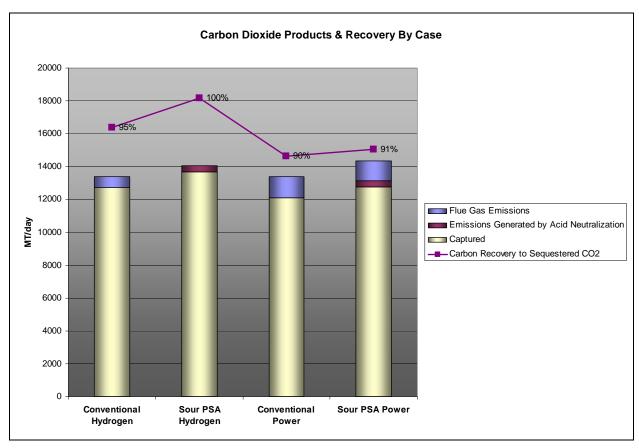
The Sour PSA cases have a clear advantage in the amount of CO<sub>2</sub> captured. This is due primarily to two factors:

- The Sour PSA technologies generate more CO<sub>2</sub> due to the addition of natural gas into the Sour Oxy-Combustor
- The conventional cases slip more CO<sub>2</sub> past the recovery section

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Although both of the sour cases generate more total  $CO_2$ , the Sour PSA power case emits slightly more than the conventional case. This is primarily due to the fact that a small amount of  $CO_2$  that is removed by the Sour PSA is added back into the gas turbine fuel as a diluent. This is a less expensive option than compressing Nitrogen from the ASU and provides for similar total capture percentages to the conventional cases. Figure 8-5 below summarizes the  $CO_2$  emissions and recovery for each of the cases.

Figure 8-5.



Note: The percentages indicated above do not include the carbon in the imported limestone.

## **Major Risks**

Any new technology has risks, especially early in the development program. One of the key issues to address for success is to understand the risks, develop mitigation strategies and potentially refocus efforts if potential "show stoppers" exist. For Air Products' Sour PSA

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technology, beyond the capex and operating cost issues there are some risks that may significantly impact the potential benefit of the Sour PSA technology. The key risk areas are as follows:

#### High Acid Neutralization Costs:

Early in the study, acid disposal costs were noted as a potential risk. During the course of the study, we concluded that neutralization was the mostly likely disposal route for the dilute acid; it was therefore included in the operating costs. Due to the costs of neutralization, there may be an incentive to produce a more concentrated sulfuric acid stream or identify less expensive disposal options. Air Products currently estimates that the sulfuric acid generated in the first stage will be dilute (40%-80%) and may contain some nitric acid as well. Although some potential off-takers of sulfuric acid (largely phosphoric acid plants associated with fertilizer production and, to a smaller extent, refiners and wallboard manufacturers) can accept lower purity sulfuric acid (maybe down to 70%), we do not know of any long range transportation occurring at concentrations below 93% due to corrosion concerns.

Acid concentration issues aside, the current sulfuric acid market may be a constraint. This single application of the Air Products acid production would likely swamp the sulfuric acid market in Western Canada, which is currently around 300,000 MT/yr (dry) and represents nearly 1% of the total North American market. Therefore, just producing a more concentrated and contaminant-free sulfuric acid stream may not improve the marketability of the acid.

#### Alternative sulfur removal technologies:

A natural outcome of the difficulties associated with sulfuric acid production is to identify and consider alternative means of sulfur removal. A side benefit of an alternative scheme would be a reduction in the capital cost associated with the acid removal equipment including compressors, all of which require enhanced metallurgy to combat the corrosive environment associated with acid production.

#### Contamination of Sour PSA with heavy metals:

Due to the absence of the Rectisol system, the Sour PSA absorbent is more susceptible to heavy metals than in a conventional process. This may require either a shutdown to resolve or more frequent absorbent replacements. One mitigation step may be to add a guard bed to absorb the heavy metals with break-through detection.

Issues related to feedstock differences or variability:

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The Sour PSA absorbent is likely more susceptible to problems related to changes in operation or gasifier feedstock that would impact composition of the Sour PSA feed, including absorbent contaminants. This may require more development work on absorbents or more frequent change-outs.

#### CO<sub>2</sub> specification changes:

The Sour PSA technology produces CO<sub>2</sub> that has a lower purity than the conventional systems. Although we opine that it is sufficient for sequestration, there may be more stringent specifications in place from future regulations. This may require further separation steps.

#### Corrosion issues:

As mentioned above, despite the enhanced metallurgy, the entire acid removal train is subject to accelerated corrosion, which may result in additional downtimes for equipment replacement or extra capital costs for more corrosion-resistant equipment.

### Recommendations

Jacobs Consultancy opines that if the Sour PSA technology performs as claimed by Air Products, there may be small but significant capital cost savings associated with eliminating the Rectisol (or Selexol) system and the sulfur recovery unit, and adding in the Sour PSA, Oxy-Combustor and Acid Removal steps. Additionally, the Sour PSA power case produces significantly more power (20 MW) than the conventional case, increasing potential revenue for the power case. The Sour PSA hydrogen case, however, produces about the same amount of hydrogen as the conventional case. Despite the capital cost benefits and production benefits, at least for the power case, significant challenges exist with respect to operating costs, largely associated with acid production and uncertainty in the capital costs associated with new equipment. Key aspects in improving Air Products' capital and operating cost while maintaining performance include:

#### Further reduction in capital costs:

Despite the elimination of two entire systems in the conventional flowschemes, the additional cost associated with the Sour PSA equipment including the Sour PSA, the Sour Oxy-Combustor and the Acid Production and Removal system provide modest cost reductions that represent 4 to 5% of the total cost of the entire gasification system. However, this capital cost advantage is less if the Sour PSA technology is evaluated in an industrial application where incremental sulfur capacity could be

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added relatively inexpensively to an existing sulfur plant associated with an upgrader or refinery.

#### Reduction in operating expense:

The operating expenses of the Sour PSA system are much higher than the conventional system due to the costs of neutralization and disposal of the sulfuric acid, which total approximately \$36 MM/yr.

#### Alternative means of sulfur component removal:

Identification and development of options related to removal of the sulfur components in the Sour PSA tailgas would reduce the operating expenses and may reduce the capital costs. Some options include PSA advancements, such as two-stage systems that would remove  $H_2S$  as well as hydrogen, and compression and co-injection of  $H_2S$  and  $CO_2$  into sequestration wells.

#### Sour PSA performance

The Sour PSA system must be robust enough to separate the hydrogen from the shifted sour gas without overly contaminating the hydrogen stream or losing a significant amount of hydrogen to the tailgas. The system must be capable of meeting the performance requirements despite changes in the feedstock occurring through gasifier feedstock variability as well as operational changes.

Once some of the cost improvements are addressed for the Sour PSA technology, other items that may be considered, if still applicable, are as follows:

#### Sour Oxy-Combustor operations:

Due to challenges associated with the low heating content fuel and oxygen firing, controlled operation of the Sour Oxy-Combustor is critical. The heating value of Sour PSA tailgas is well below 80 BTU/SCF, and, therefore, natural gas is added to bring up the heating value to 80 BTU/SCF. Control of the natural gas and ultimate heating value will be critical to maintain a flame in the sour combustor. Similarly, control of the pressurized oxygen will be critical to keep the operation safe and reliable.

#### Sour flue gas compression and acid production:

Although we do not doubt the chemistry of the reactions proposed by Air Products, there are real world challenges to the commercial operation, and care must be taken in the design to ensure that the acids are generated and the contaminants removed from the CO<sub>2</sub> stream. The first challenge is to ensure that the sulfuric acid—and to a

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lesser extent, the nitric acid—is produced, removing the  $SO_2$  and  $NO_x$  components from the flue gas. This involves not only the kinetics but equilibrium of the reactions, which may be much different in a plug flow system than a bench top scale CSTR. The second challenge involves the metallurgy of the entire system, extending from cooling of the flue gas to condensation temperatures, compression, additional cooling, pumps and vessels. It is known that dilute sulfuric acid is very corrosive, and maintaining mechanical integrity is critical and sometimes costly.

#### Successful integration of heat available from the Sour Oxy-Combustor:

Based on our evaluation of the gasification/power block operation, we opine that superheating some of the steam produced in the gasifier, in addition to steam generation, will maximize the efficiency of the integrated system, but further optimization on a case-by-case basis is possible, including preheating of gasifier feedstocks, increasing the temperature of the gas turbine fuel, or heat recovery in another industrial application.

#### Gasifier technology selection:

For the purposes of the commercial feasibility, we assumed a conventional GE slurry-fed gasifier operating in total quench. Further work will be necessary to evaluate the various gasifier licensor offerings to maximize the advantages of the Sour PSA technology.

#### Evaluation of Sour PSA technology in other applications:

As previously alluded to, the benefits of the Air Products technology will be different depending on the application. For example, if the entire gasifier block was integrated with a refinery or upgrader, which is likely since the technology uses a petcoke feed and produces hydrogen, then arrangements could be made to process the H<sub>2</sub>S generated in a conventional Rectisol/Selexol system via expansion of the Sulfur Recovery Unit operated by the Upgrader/ Refinery.

Alternatively, the Sour PSA technology might show larger benefits compared to a conventional technology for low sulfur feedstocks where the neutralization costs could be reduced. Likewise, evaluation of the technology for gasifiers aimed at producing petrochemical feedstocks or Fischer-Tropsch feedstocks may show different benefits.

#### Evaluation of other technologies for synergy:

Other technologies may provide a synergistic benefit for H<sub>2</sub>S removal, including Electrical Swing Absorption (ESA), Carbon Fiber Composite Molecular Sieves (CFCMS) or membranes.

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#### Full quantification of risks:

As part of the study, a semi-quantitative evaluation of the technical risks was completed. We often find benefits with full project value risk quantification taking into consideration uncertainty related to Capex, Opex, project implementation schedule, Product-Feed price spreads, regulatory issues, technology performance/unit availability, Forex, inflation, market size and growth rates, competitive response, and HS&E issues.

#### Utility impacts and other emissions:

Our current level of analysis indicates that the Sour PSA schemes use more water than the conventional schemes and also produce more solid and liquid emissions. Further study may identify ways to reduce the impact of both.

# Appendix 1.

# **Options for Flowscheme Selection**

### Options for Flowscheme Selection

**Table 1. Results of Jacobs Consultancy Internal Brainstorming Session** 

Preheat power block fuel to 100°F using hot condensate of LP steam, not in oxy-combustor  1 oxy-combustor  No High  No Way sump process streams to preheat power block feeds  Do not premix N2 and H2 prior to power block  May supplement N2 in power block with steam  No Medium  Use multiple steam turbines in the power block for LP and HP steam  Essaturator heat removal generating LP steam rather than Rectisol  reboiling  Do not cool process water recycled back to coke slurry  Use single stage shift rather than two-stage to save capital  Use of the oxyfuel combustor heat to superheat steam at various pressures  rather than making only saturated steam  Use of a condensing economizer after oxy-combustor convection section to recover heat  Increased tailgas pressure to reduce compression costs; trade-off is lower recover within the PSA and higher pressure oxyfuel combustion  Place fuel gas expander upstream of PSA unit  Place fuel fuel			AP Tech Only?	Rank
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Increased tailgas pressure to reduce compression costs; trade-off is lower recovery within the PSA and higher pressure oxyfuel combustion Yes High Place fuel gas expander upstream of PSA unit Yes Low Maintain 3 ppm H2S maximum to power block, consistent with Selexol guaranteed value (Rectisol is lower) Yes Low Use of an O2 scavenging bed to remove inerts from CO2 rather than using cold box (if inert removal is required) Yes High Development of a design for less stringent sequestration specs, not for Enhanced Oil Recovery (EOR) Yes High Use knockout drum rather than contactor for second stage discharge if acid is not present Yes Medium Review compressor technology selection for efficiency Yes Medium Neutralization and landspreading / landfilling of dilute acids Yes High Mercury removal before the Sour PSA or membrane WESP (claims to remove Hg) Yes High Wet limestone scrubbing of oxy-combustor flue gas Yes High Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, then recompress, at high cost Yes Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of				
recovery within the PSA and higher pressure oxyfuel combustion  Place fuel gas expander upstream of PSA unit  Place fuel gas expander upstream of PSA unit  Maintain 3 ppm H2S maximum to power block, consistent with Selexol  guaranteed value (Rectisol is lower)  Use of an O <sub>2</sub> scavenging bed to remove inerts from CO <sub>2</sub> rather than using  cold box (if inert removal is required)  Pevelopment of a design for less stringent sequestration specs, not for  Penhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid  is not present  Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Neutralization and landspreading / landfilling of dilute acids  Pes  Medium  Nercury removal before the Sour PSA or membrane WESP (claims to  remove Hg)  Yes  High  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  then recompress, at high cost  Pes  Yes  Low  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	12		Yes	High
14 Place fuel gas expander upstream of PSA unit  Maintain 3 ppm H2S maximum to power block, consistent with Selexol  15 guaranteed value (Rectisol is lower)  Use of an O <sub>2</sub> scavenging bed to remove inerts from CO <sub>2</sub> rather than using  16 cold box (if inert removal is required)  Development of a design for less stringent sequestration specs, not for  17 Enhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid  18 is not present  Yes  Medium  19 Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to  21 remove Hg)  Yes  High  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of				
Maintain 3 ppm H2S maximum to power block, consistent with Selexol  15 guaranteed value (Rectisol is lower)  Use of an O <sub>2</sub> scavenging bed to remove inerts from CO <sub>2</sub> rather than using  16 cold box (if inert removal is required)  Development of a design for less stringent sequestration specs, not for  17 Enhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid  18 is not present  Yes  Medium  19 Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to  21 remove Hg)  Yes  High  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  then recompress, at high cost  Yes  Low  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of		,		Ŭ
Use of an O <sub>2</sub> scavenging bed to remove inerts from CO <sub>2</sub> rather than using cold box (if inert removal is required)  Development of a design for less stringent sequestration specs, not for Enhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid is not present  Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to remove Hg)  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	14		Yes	Low
Use of an O <sub>2</sub> scavenging bed to remove inerts from CO <sub>2</sub> rather than using 16 cold box (if inert removal is required)  Development of a design for less stringent sequestration specs, not for 17 Enhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid 18 is not present  Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to 18 remove Hg)  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 19 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	4-			
16 cold box (if inert removal is required) Development of a design for less stringent sequestration specs, not for Enhanced Oil Recovery (EOR) Use knockout drum rather than contactor for second stage discharge if acid 18 is not present Yes Medium 19 Review compressor technology selection for efficiency Neutralization and landspreading / landfilling of dilute acids Mercury removal before the Sour PSA or membrane WESP (claims to 11 remove Hg) Yes High Wet limestone scrubbing of oxy-combustor flue gas Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 14 then recompress, at high cost Tyes Low Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	15	guaranteed value (Rectisol is lower)	Yes	Low
Development of a design for less stringent sequestration specs, not for 17 Enhanced Oil Recovery (EOR)  Use knockout drum rather than contactor for second stage discharge if acid 18 is not present  Yes  Medium 19 Review compressor technology selection for efficiency  Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to 21 remove Hg)  Yes  High  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 23 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	16		Yes	High
17 Enhanced Oil Recovery (EOR) Use knockout drum rather than contactor for second stage discharge if acid 18 is not present Yes Medium 19 Review compressor technology selection for efficiency Neutralization and landspreading / landfilling of dilute acids Mercury removal before the Sour PSA or membrane WESP (claims to 21 remove Hg) Yes High Wet limestone scrubbing of oxy-combustor flue gas Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 23 then recompress, at high cost Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	10	. ,	100	i ligii
Use knockout drum rather than contactor for second stage discharge if acid is not present Yes Medium Review compressor technology selection for efficiency Neutralization and landspreading / landfilling of dilute acids Mercury removal before the Sour PSA or membrane WESP (claims to remove Hg) Yes High Wet limestone scrubbing of oxy-combustor flue gas Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, then recompress, at high cost Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	17		Yes	High
18 is not present 19 Review compressor technology selection for efficiency 20 Neutralization and landspreading / landfilling of dilute acids 21 remove Hg) 22 Wet limestone scrubbing of oxy-combustor flue gas 23 Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 23 then recompress, at high cost 24 Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of			. 00	g
19 Review compressor technology selection for efficiency 20 Neutralization and landspreading / landfilling of dilute acids 21 remove Hg) 22 Wet limestone scrubbing of oxy-combustor flue gas 23 Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 23 then recompress, at high cost 24 Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	18		Yes	Medium
20 Neutralization and landspreading / landfilling of dilute acids  Mercury removal before the Sour PSA or membrane WESP (claims to 21 remove Hg)  Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of		•		Medium
Mercury removal before the Sour PSA or membrane WESP (claims to 21 remove Hg) 22 Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust, 23 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of		,	Yes	
21 remove Hg) 22 Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  23 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of		·		J
22 Wet limestone scrubbing of oxy-combustor flue gas  Amine-treat tailgas for H2S removal when unit is part of an upgrader which already has a Claus plant; must compress first, than expand to combust,  23 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	21		Yes	High
already has a Claus plant; must compress first, than expand to combust,  23 then recompress, at high cost  Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	22	Wet limestone scrubbing of oxy-combustor flue gas	Yes	High
Rectisol (one step) treat Sour PSA feed for H2S removal when unit is part of	23	already has a Claus plant; must compress first, than expand to combust,	Vas	Low
	23		163	LOW
	24		Yes	Low

# Table 2. Additional Flowscheme Options by Jacobs Consultancy & Air Products

Elimination of the cold box—no inerts removal

First stage of compression upstream of the oxyfuel combustion

Other uses for acids (fertilizer, ammonia, etc.)

Use of ash from nearby power plant for acid neutralization (conventional pulverization)

Use of the low-grade heat generated in the oxy-combustor and gasification sections for acid concentration

Two-stage PSA: first stage CO2 rejection, second stage for H2 purity

Two-stage PSA: first stage H2S removal to Claus unit, second stage for H2 purity

Two-stage PSA: Within an upgrader, use the first PSA to achieve the power block feed composition

(within the H2S limits), and the second PSA to get product H2 purity

Purge the PSA with CO2 instead of H2 for higher CO2 purity

Purge the PSA with N2

Licensed ammonia scrubber technology to convert SO2 to ammonium sulfate for fertilizer

Licensed technology to treat the flue gas by converting SO2 to concentrated, high-purity sulfuric acid

and converting NOx to N2

# Appendix 2.

# **Block Flow Diagrams for Each Case**

Figure 1.
Block Flow Diagram for Conventional Hydrogen Production Case

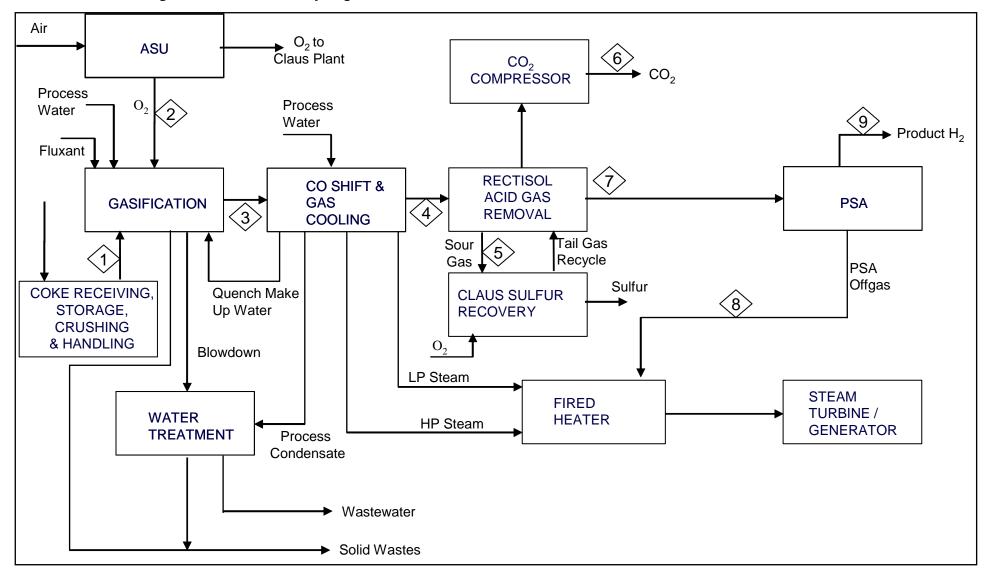


Figure 2.
Block Flow Diagram for Conventional Power Generation Case

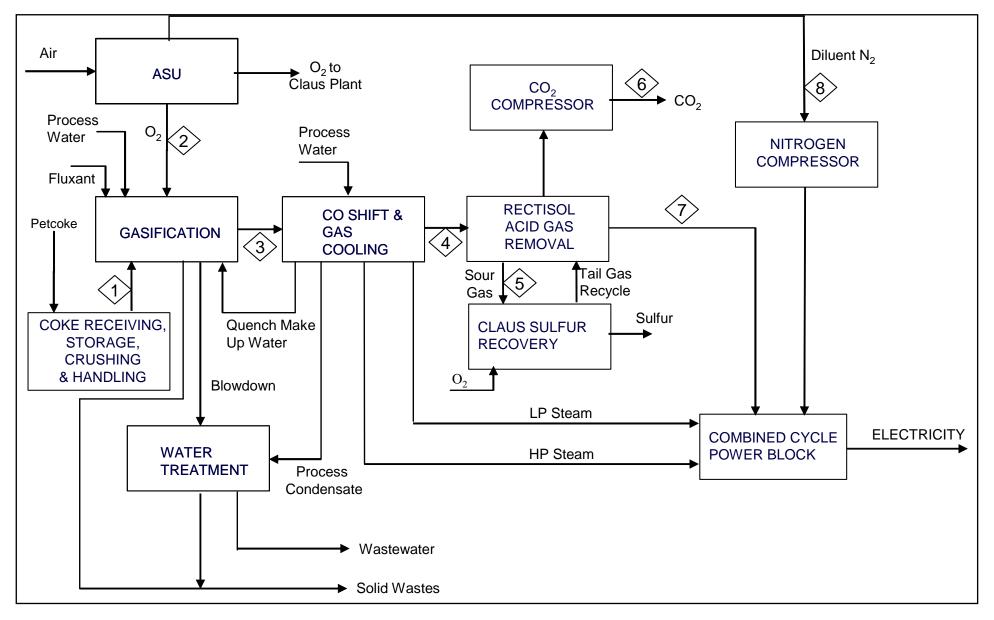


Figure 3.
Block Flow Diagram for Sour PSA Hydrogen Production Case

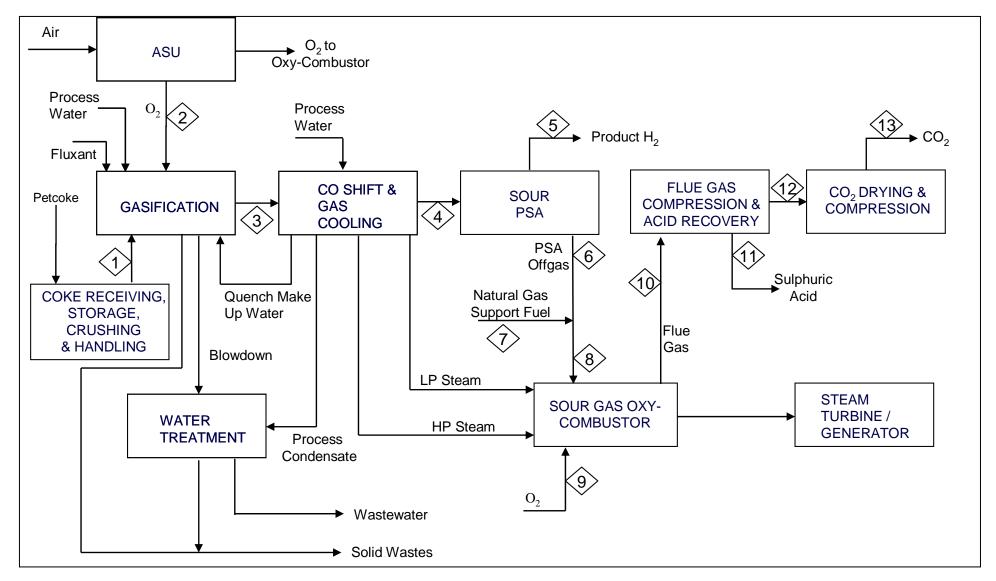
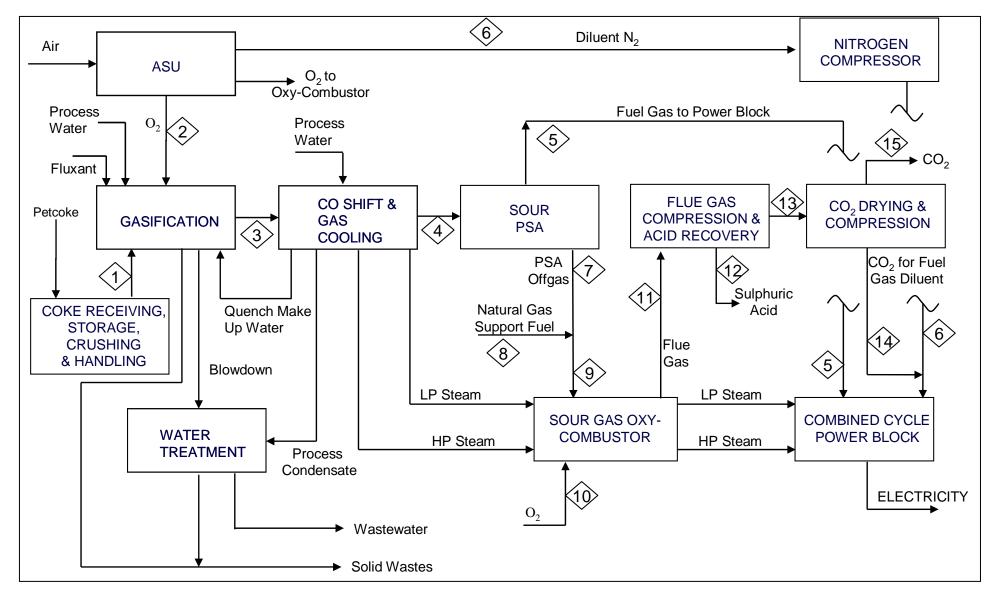


Figure 4.
Block Flow Diagram for Sour PSA Power Generation Case



# Appendix 3.

# **Heat & Material Balances**

Table 1. Heat and Material Balance for Conventional Hydrogen Production Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR28	300/P03	3/1001					
CONSULTANCY		МΔ	SSR	ALAN	JCF		Project No.	:	61LR2800		Plant:		SE HYDR			
							Client	:	AIR PROI	DUCTS	Location:	EDMONT	ON, ALBE	RTA		
The information contained herein is is issued on the understanding that							Case	Case : 4,472.5 tonnes/day petcoke gasification								
JACOBS ENGINEERING UK LTD. Toontract.							Case	:	for hydro		-	gasilicati	OII			
STREAM NUMBER			1		2		<u>1</u> 3		Ba		Bb		3c		3d	
STREAM NAME		PETO	OKF	GASIFICA		GASIFICA	~		r reactor	SHIFT RE			EACTOR 2		EACTOR 2	
		FEEDS			N FEED		ICT GAS		ED		UENT		ED		UENT	
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	
Hydrogen	2.016	0	0.00	0	0.00	7,028	34.63	7,028	34.63	14,949	52.94	14,949	52.94	15,614	54.02	
Nitrogen	28.013	0	0.00	0	0.00	92	0.45	92	0.45	92	0.32	92	0.32	92	0.32	
Carbon Monoxide	28.010	0	0.00	0	0.00	8,954	44.12	8,954	44.12	1,033	3.66	1,033	3.66	368	1.27	
Carbon Dioxide	44.010	0	0.00	0	0.00	3,794	18.70	3,794	18.70	11,740	41.57	11,740	41.57	12,406	42.92	
Methane	16.043	0	0.00	0	0.00	13	0.07	13	0.07	13	0.05	13	0.05	13	0.05	
Argon	39.948	0	0.00	31	0.50	31	0.15	31	0.15	31	0.11	31	0.11	31	0.11	
Hydrogen Sulphide	34.080	0	0.00	0	0.00	352	1.74	352	1.74	377	1.34	377	1.34	378	1.31	
Carbonyl Sulphide	60.070	0	0.00	0	0.00	26	0.13	26	0.13	2	0.01	2	0.01	1	0.00	
Ammonia	17.030	0	0.00	0	0.00	4	0.02	4	0.02	4	0.01	4	0.01	4	0.01	
Oxygen	31.999	0	0.00	6,131	99.50	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Petcoke (tonnes/day)		4,472.5 (1)														
Temperature	°C	25		121		247		290		429		300		312		
Pressure	bara	1.00		83.34		67.86		67.56		67.16		66.56		66.16		
Total Dry Molar Flow (km	nol/h, %)	-	-	6,162	100.00	20,294	2.04	20,294	2.04	28,240	1.46	28,240	1.46	28,906	1.43	
Water (kmol/h)	18.015	-		0		32,688		32,688		24,742		24,742		24,076		
TOTAL WET (kmol/h)		_		6,162		52,982		52,982		52,982		52,982		52,982		
Total Mass Flow (kg/h)		186,356	(Note 1)	197	,429	1,03	8,497	1,03	8,497	1,03	8,497	1,03	8,497	1,03	8,497	
Molecular Weight				32	2.0	19	9.6	19	9.6	19	9.6	19.6		19	9.6	
Notes :	Notes :		Issue:	Α	Date	В	Date		Date		Date		Date		Page	
Stated mass flow rep	Stated mass flow represents dry basis.  Description:			FOR STUDY HEAT I		DETAIL		,						1		
	As received coke contains 12% w/w H <sub>2</sub> O.			ARA	29-Jan-09	LEW	16-Apr-09								of	
	-														2	
		Checked: Approved:										i e		1 -		

Table 1 cont'd. Heat and Material Balance for Conventional Hydrogen Production Case

<b>JACOBS</b>	,	JACOBS	CONSU	ILTANC'	Y UK LTI	)	Document No.	012112000/1001										
CONSULTANCY		МА	SS B	ΔΙ ΔΝ	ICE		Project No.	:	61LR280		Plant:		ASE HYDR					
							Client	:	AIR PRO	DUCTS	Location:	EDMON	ΓON, ALBE	RTA				
is issued on the understanding that	e information contained herein is confidential, the property of JACOBS ENGINEERING UK LTD, and not for publication. The information issued on the understanding that no part thereof shall be copied or communicated to a third party without authorisation in writing from COBS ENGINEERING UK LTD. The data contained in this document is subject to change during the design stage of any subsequent ntract.							:		onnes/day gen prod		gasificat	ion					
STREAM NUMBER			е		4		5		6		7		8		9			
STREAM NAME		DESATU FE	JRATOR ED	AGR UN	IIT FEED	SOUF	R GAS	CO <sub>2</sub> TO	EXPORT	TREATED	SYNGAS		FGAS TO L GAS		OGEN DUCT			
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)			
Hydrogen	2.016	15,614	54.02	15,601	54.24	0	0.00	46	0.38	15,555	95.41	1,989	73.03	13,566	99.90			
Nitrogen	28.013	92	0.32	92	0.32	2	0.39	1	0.01	91	0.56	91	3.35	0	0.00			
Carbon Monoxide	28.010	368	1.27	367	1.28	0	0.00	1	0.01	366	2.25	366	13.45	0	0.00			
Carbon Dioxide	44.010	12,406	42.92	12,297	42.76	259	41.64	12,053	99.60	246	1.51	246	9.03	0	0.00			
Methane	16.043	13	0.05	13	0.05	0	0.00	0	0.00	13	0.08	13	0.47	0	0.00			
Argon	39.948	31	0.11	31	0.11	0	0.00	0	0.00	31	0.19	18	0.67	13	0.10			
Hydrogen Sulphide	34.080	378	1.31	359	1.25	360	57.86	0	0.00	0	0.00	0	0.00	0	0.00			
Carbonyl Sulphide	60.070	1	0.00	1	0.00	1	0.11	0	0.00	0	0.00	0	0.00	0	0.00			
Ammonia	17.030	4	0.01	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00			
Oxygen	31.999	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00			
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00			
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00			
Petcoke (tonnes/day)																		
Temperature	°C	257		44		44		37		44		43		44				
Pressure	bara	65.56		65.00		65.00		152.00		64.70		1.30		64.70				
Total Dry Molar Flow (km	nol/h, %)	28,906	100.00	28,760	100.00	622	100.00	12,101	100.00	16,303	100.00	2,724	100.00	13,579	100.00			
Water (kmol/h)	18.015	24,076		48		0		0		0		0		0				
TOTAL WET (kmol/h)		52,982		28,808		622		12,101		16,303		2,724		13,579				
Total Mass Flow (kg/h)		1,03	3,497	600	,065	23,	771	530	,622	56,	462	28	,586	27,	877			
Molecular Weight		19	).6	20	0.8	38	3.2	43	3.8	3	.5	1	0.5	2	.1			
Notes :			Issue:	Α	Date	В	Date		Date		Date		Date		Page			
1. Hydrogen production	Hydrogen production = 272.6 mmscfd.		Description:	FOR STUDY		HEAT DETAIL									2			
	, , ,			ARA	29-Jan-09	LEW	16-Apr-09								of			
															2			

Table 2. Heat and Material Balance for Conventional Power Generation Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No. : 61LR2800/P03/1001									
		М	SS B	ALAN	ICE		Project No.	:	61LR2800		Plant:		SE POWE			
CONSULTANCY		IVI	133 D		ICL		Client : AIR PRODUCTS Location: EDMONTON, ALBERTA									
The information contained herein is is issued on the understanding that																
JACOBS ENGINEERING UK LTD.							Case	Case : 4,472.5 tonnes/day petcoke gasification								
contract.				1		1		•	for powe	r producti	ion					
STREAM NUMBER		•	'		2		3		Ва		Bb		3c		3d	
STREAM NAME		PETO		GASIFICA		GASIFICA			REACTOR	SHIFT RE			EACTOR 2	_	EACTOR 2	
		FEEDS			N FEED		CT GAS		ED		UENT		ED		UENT	
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	
Hydrogen	2.016	0	0.00	0	0.00	7,026	34.13	7,026	34.13	14,962	52.41	14,962	52.41	15,617	53.48	
Nitrogen	28.013	0	0.00	129	2.00	220	1.07	220	1.07	220	0.77	220	0.77	220	0.75	
Carbon Monoxide	28.010	0	0.00	0	0.00	8,953	43.50	8,953	43.50	1,017	3.56	1,017	3.56	363	1.24	
Carbon Dioxide	44.010	0	0.00	0	0.00	3,794	18.43	3,794	18.43	11,755	41.18	11,755	41.18	12,410	42.50	
Methane	16.043	0	0.00	0	0.00	13	0.06	13	0.06	13	0.05	13	0.05	13	0.05	
Argon	39.948	0	0.00	194	3.00	194	0.94	194	0.94	194	0.68	194	0.68	194	0.66	
Hydrogen Sulphide	34.080	0	0.00	0	0.00	352	1.71	352	1.71	377	1.32	377	1.32	378	1.29	
Carbonyl Sulphide	60.070	0	0.00	0	0.00	26	0.13	26	0.13	2	0.01	2	0.01	1	0.00	
Ammonia	17.030	0	0.00	0	0.00	6	0.03	6	0.03	6	0.02	6	0.02	6	0.02	
Oxygen	31.999	0	0.00	6,131	95.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	
Petcoke (tonnes/day)		4,472.5 (1)														
Temperature	°C	25		121		246		290		428		300		311		
Pressure	bara	1.00		83.34		67.86		67.56		67.16		66.56		66.16		
Total Dry Molar Flow (km	nol/h, %)	-	-	6,454	100.00	20,584	100.00	20,584	100.00	28,545	100.00	28,545	100.00	29,201	100.00	
Water (kmol/h)	18.015	-		0		32,949		32,949		24,988		24,988		24,332		
TOTAL WET (kmol/h)		-		6,454		53,533		53,533		53,533		53,533		53,533		
Total Mass Flow (kg/h)		186,356	(Note 1)	207	,550	1,05	3,305	1,05	3,305	1,05	3,305	1,05	3,305	1,05	3,305	
Molecular Weight	Molecular Weight -			32	2.2	19	9.7	19	9.7	19.7		19.7		19	9.7	
Notes :	Notes :		Issue:	Α	Date	В	Date		Date		Date		Date		Page	
1. Stated mass flow rep	Stated mass flow represents dry basis.  Descr			: FOR STUDY HEAT		HEAT	DETAIL		,						1	
As received coke cor	ntains 12%	w/w H <sub>2</sub> O.	Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of	
	-														2	
			Checked: Approved:												1	

Table 2 cont'd. Heat and Material Balance for Conventional Power Generation Case

<b>JACOBS</b>	,	JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR2	800/P03	3/1001				
CONSULTANCY		MΔ	SS B	ΔΙ ΔΝ	ICF		Project No.	:	61LR2800		Plant:		SE POWE		
							Client	:	AIR PROI	DUCTS	Location:	EDMONT	ON, ALBE	RTA	
is issued on the understanding that	The information contained herein is confidential, the property of JACOBS ENGINEERING UK LTD, and not for publication. The information is issued on the understanding that no part thereof shall be copied or communicated to a third party without authorisation in writing from IACOBS ENGINEERING UK LTD. The data contained in this document is subject to change during the design stage of any subsequent contract.									onnes/day	•	gasificati	on		
STREAM NUMBER		3	se		4		5		6	•	7		8		
STREAM NAME			JRATOR ED	AGR UN	IIT FEED	SOUF	R GAS	CO <sub>2</sub> TO	EXPORT		GAS TO R BLOCK		N DILUENT ER BLOCK		
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	15,617	53.48	15,603	53.70	0	0.00	46	0.40	15,557	90.44	0	0.00		
Nitrogen	28.013	220	0.75	220	0.76	6	0.92	2	0.01	215	1.25	12,550	99.30		
Carbon Monoxide	28.010	363	1.24	362	1.25	0	0.00	1	0.01	361	2.10	0	0.00		
Carbon Dioxide	44.010	12,410	42.50	12,302	42.34	256	41.11	11,446	99.56	862	5.01	0	0.00		
Methane	16.043	13	0.05	13	0.05	0	0.00	0	0.00	13	0.07	0	0.00		
Argon	39.948	194	0.66	193	0.67	0	0.00	2	0.01	193	1.12	88	0.70		
Hydrogen Sulphide	34.080	378	1.29	359	1.24	360	57.86	0	0.00	0	0.00	0	0.00		
Carbonyl Sulphide	60.070	1	0.00	1	0.00	1	0.11	0	0.00	0	0.00	0	0.00		
Ammonia	17.030	6	0.02	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Oxygen	31.999	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		<u> </u>
Petcoke (tonnes/day)															
Temperature	°C	257		48		47		37		47		15			
Pressure	bara	65.56		65.00		65.00		152.00		64.70		1.01			
Total Dry Molar Flow (kn	nol/h, %)	29,201	100.00	29,054	100.00	622	100.00	11,496	100.00	17,201	100.00	12,638	100.00		
Water (kmol/h)	18.015	24,332		57		0		0		0		0			
TOTAL WET (kmol/h)		53,533		29,111		622		11,496		17,201		12,638			
Total Mass Flow (kg/h)		1,05	3,305	610	,420	23,	723	503	3,980	93,	336	355	5,104		
Molecular Weight		19	9.7	2	1.0	38	3.1	43	3.8	5	.4	2	8.1		
Notes :			Issue:	Α	Date	В	Date		Date		Date		Date		Page
			Description:	: FOR STUDY		HEAT DETAIL									2
				ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												2
	Approved:												1		

Table 3. Heat and Material Balance for Sour PSA Hydrogen Production Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR2	300/P03	3/1001				
0110000		МΛ	SS B	ALAN	JCE		Project No.	:	61LR2800		Plant:		SA HYDRO		
CONSULTANCY							Client	:	AIR PROI	DUCTS	Location:	EDMONT	ON, ALBE	RTA	
The information contained herein is is issued on the understanding that							0		4 470 E 4						
JACOBS ENGINEERING UK LTD							Case	:	4,472.5 to	_	•	gasificati	on		
					0		<u> </u>		for hydro	<u> </u>			2 -		) -l
STREAM NUMBER STREAM NAME		PETC	OVE	GASIFICA	ZION LINIT	GASIFICA	3		3a FREACTOR	SHIFT RE	Sb CTOP 4		3c EACTOR 2		EACTOR 2
STREAM NAME		FEEDS			N FEED		CT GAS		ED	EFFL			ED EACTOR 2	_	UENT
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	0	0.00	0	0.00	7,028	34.63	7,028	34.63	14,949	52.94	14,949	52.94	15,614	54.02
Nitrogen	28.013	0	0.00	0	0.00	92	0.45	92	0.45	92	0.32	92	0.32	92	0.32
Carbon Monoxide	28.010	0	0.00	0	0.00	8,954	44.12	8,954	44.12	1,033	3.66	1,033	3.66	368	1.27
Carbon Dioxide	44.010	0	0.00	0	0.00	3,794	18.70	3,794	18.70	11,740	41.57	11,740	41.57	12,406	42.92
Methane	16.043	0	0.00	0	0.00	13	0.07	13	0.07	13	0.05	13	0.05	13	0.05
Argon	39.948	0	0.00	31	0.50	31	0.15	31	0.15	31	0.11	31	0.11	31	0.11
Hydrogen Sulphide	34.080	0	0.00	0	0.00	352	1.74	352	1.74	377	1.34	377	1.34	378	1.31
Carbonyl Sulphide	60.070	0	0.00	0	0.00	26	0.13	26	0.13	2	0.01	2	0.01	1	0.00
Ammonia	17.030	0	0.00	0	0.00	4	0.02	4	0.02	4	0.01	4	0.01	4	0.01
Oxygen	31.999	0	0.00	6,131	99.50	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Petcoke (tonnes/day)		4,472.5 (1)													
Temperature	°C	25		121		247		290		429		300		312	
Pressure	bara	1.00		83.34		67.86		67.56		67.16		66.56		66.16	
Total Dry Molar Flow (km	nol/h, %)	-	-	6,162	100.00	20,294	100.00	20,294	100.00	28,240	100.00	28,240	100.00	28,906	100.00
Water (kmol/h)	18.015			0		32,690		32,690		24,744		24,744		24,078	
TOTAL WET (kmol/h)		-		6,162		52,984		52,984		52,984		52,984		52,984	
Total Mass Flow (kg/h)	al Mass Flow (kg/h) 186,3			197	,429	1,03	8,531	1,03	8,531	1,03	8,531	1,03	8,531	1,03	8,531
Molecular Weight	ecular Weight			32	2.0	19	9.6	19	9.6	19	9.6	1	9.6	19	9.6
Notes :				Α	Date	В	Date		Date		Date		Date		Page
Stated mass flow rep	resents dry	basis.	Description:	FOR	STUDY	HEAT	DETAIL								1
As received coke cor			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:						1				1		1

Table 3 cont'd. Heat and Material Balance for Sour PSA Hydrogen Production Case

<b>JACOBS</b>	,	JACOBS	CONSU	ILTANC'	Y UK LTI	)	Document No.	:	61LR2	800/P03	3/1001				
		МА	SS B	ΔΙ ΔΝ	ICE		Project No.	:	61LR2800		Plant:		SA HYDRO	_	
CONSULTANCY							Client	:	AIR PROI	DUCTS	Location:	EDMONT	TON, ALBE	RTA	
The information contained herein is is issued on the understanding that I JACOBS ENGINEERING UK LTD. T contract.	no part thereof s	hall be copied or	communicated to	a third party with	out authorisation i	n writing from	Case	:	4,472.5 to	•	•	gasificati	ion		
STREAM NUMBER		3	е		4	į	5		6		7		8		9
STREAM NAME			JRATOR ED	SOUR P	SA FEED		OGEN DUCT		FGAS TO MBUSTOR		MBUSTOR RT FUEL		MBUSTOR D FUEL		MBUSTOR EN FEED
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	15,614	54.02	15,601	54.24	13,361	99.96	2,240	14.55	0	0.00	2,240	14.34	0	0.00
Nitrogen	28.013	92	0.32	92	0.32	0	0.00	91	0.59	0	0.00	91	0.58	0	0.00
Carbon Monoxide	28.010	368	1.27	367	1.28	0	0.00	367	2.39	0	0.00	367	2.35	0	0.00
Carbon Dioxide	44.010	12,406	42.92	12,297	42.76	0	0.00	12,297	79.88	0	0.00	12,297	78.73	0	0.00
Methane	16.043	13	0.05	13	0.05	0	0.00	13	0.09	225	100.00	238	1.52	0	0.00
Argon	39.948	31	0.11	31	0.11	6	0.04	25	0.16	0	0.00	25	0.16	13	0.50
Hydrogen Sulphide	34.080	378	1.31	359	1.25	0	0.00	359	2.33	0	0.00	359	2.30	0	0.00
Carbonyl Sulphide	60.070	1	0.00	1	0.00	0	0.00	1	0.00	0	0.00	1	0.00	0	0.00
Ammonia	17.030	4	0.01	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Oxygen	31.999	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	2,510	99.50
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Petcoke (tonnes/day)															
Temperature	°C	257		44		44		44		25		44		25	
Pressure	bara	65.56		65.00		64.29		1.30		1.30		1.30		2.00	
Total Dry Molar Flow (km	nol/h, %)	28,906	100.00	28,760	100.00	13,367	100.00	15,393	100.00	225	100.00	15,618	100.00	2,522	100.00
Water (kmol/h)	18.015	24,078		48		0		25		0		25		0	
TOTAL WET (kmol/h)		52,984		28,808		13,367		15,419		225		15,643		2,522	
Total Mass Flow (kg/h)	al Mass Flow (kg/h) 1,0			600	,065	27,	162	572	2,495	3,6	604	576	6,100	80	,810
Molecular Weight	( ) /			20	0.8	2	.0	37	7.1	16	3.0	3	6.8	3.	2.0
Notes :	· ·			Α	Date	В	Date		Date		Date		Date		Page
1. Hydrogen production	= 268.4 mi	mscfd.	Description:	FOR S	STUDY	HEAT	DETAIL								2
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:												

Table 3 cont'd. Heat and Material Balance for Sour PSA Hydrogen Production Case

<b>JACOBS</b>		JACOBS	CONSU	ILTANC'	Y UK LTI	)	Document No.	:	61LR2	800/P03	3/1001				
		МА	SS B	$\Lambda$ I $\Lambda$ N			Project No.	:	61LR280		Plant:	SOUR PS	SA HYDRO	GEN	
CONSULTANCY		IVI	133 D	ALAI	1CL		Client	:	AIR PRO	DUCTS	Location:	<b>EDMONT</b>	TON, ALBE	RTA	
The information contained herein is is issued on the understanding that JACOBS ENGINEERING UK LTD. Toontract.	no part thereof s	hall be copied or	communicated to	a third party with	nout authorisation i	n writing from	Case	:		onnes/day gen prod	•	gasificati	ion		
STREAM NUMBER		1	0	1	11	1	2	1	13	1	4		15	,	16
STREAM NAME		SOUR CO	MBUSTOR GAS		RIC ACID DUCT		ED FLUE AS	CO <sub>2</sub> TO	EXPORT	SOUR CO	MBUSTOR BFW		MBUSTOR STEAM	_	RXR HP EAM
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Nitrogen	28.013	91	0.67	0	0.00	91	0.69	91	0.69	0	0.00	0	0.00	0	0.00
Carbon Monoxide	28.010	1	0.01	0	0.00	1	0.01	1	0.01	0	0.00	0	0.00	0	0.00
Carbon Dioxide	44.010	12,901	94.98	0	0.00	12,901	97.56	12,901	97.56	0	0.00	0	0.00	0	0.00
Methane	16.043	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Argon	39.948	38	0.28	0	0.00	38	0.29	38	0.29	0	0.00	0	0.00	0	0.00
Hydrogen Sulphide	34.080	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Carbonyl Sulphide	60.070	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Ammonia	17.030	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Oxygen	31.999	191	1.41	0	0.00	191	1.45	191	1.45	0	0.00	0	0.00	0	0.00
Sulphur Dioxide	64.063	360	2.65	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphuric Acid	98.078	0	0.00	360	100.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Petcoke (tonnes/day)															
Temperature	°C	200		30		30		30		30		286		286	
Pressure	bara	1.04		1.01		29.80		152.00		75.00		70.00		70.00	
Total Dry Molar Flow (km	nol/h, %)	13,583	100.00	360	100.00	13,223	100.00	13,223	100.00	0	0.00	0	0.00	0	0.00
Water (kmol/h)	18.015	3,100		0		0		0		9,258		8,888		8,580	
TOTAL WET (kmol/h)		16,683		360		13,223		13,223		9,258		8,888		8,580	
Total Mass Flow (kg/h)	al Mass Flow (kg/h) 65			35,	296	578	,003	578	,003	166	,793	160	),121	154	1,563
Molecular Weight	( 3 /			98	3.1	43	3.7	43	3.7	18	3.0	1	8.0	18	8.0
Notes :					Date	В	Date		Date		Date		Date		Page
			Description:	FOR S	STUDY	HEAT	DETAIL								3
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:												1

Table 3 cont'd. Heat and Material Balance for Sour PSA Hydrogen Production Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR28						
		МА	SS B	ΔΙ ΔΝ	ICE		Project No.	:	61LR2800				SA HYDRO		
CONSULTANCY							Client	:	AIR PRO	DUCTS	Location:	EDMON <sup>-</sup>	TON, ALBE	RTA	
The information contained herein is is issued on the understanding that JACOBS ENGINEERING UK LTD. 1 contract.	no part thereof s	hall be copied or	communicated to	a third party with	nout authorisation i	n writing from	Case	:	4,472.5 to		y petcoke (	gasificat	ion		
STREAM NUMBER		1	7	1	18	1	19								
STREAM NAME			SUPER HP STEAM		MBUSTOR TEAM		EATED LP EAM								
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	0	0.00	0	0.00	0	0.00								
Nitrogen	28.013	0	0.00	0	0.00	0	0.00								
Carbon Monoxide	28.010	0	0.00	0	0.00	0	0.00								
Carbon Dioxide	44.010	0	0.00	0	0.00	0	0.00								
Methane	16.043	0	0.00	0	0.00	0	0.00								
Argon	39.948	0	0.00	0	0.00	0	0.00								
Hydrogen Sulphide	34.080	0	0.00	0	0.00	0	0.00								
Carbonyl Sulphide	60.070	0	0.00	0	0.00	0	0.00								
Ammonia	17.030	0	0.00	0	0.00	0	0.00								
Oxygen	31.999	0	0.00	0	0.00	0	0.00								
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00								
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00						1		<u> </u>
Petcoke (tonnes/day)															+
Temperature	°C	700		160		360									
Pressure	bara	65.00		6.00		5.50									
Total Dry Molar Flow (km	nol/h, %)	0	0.00	0	0.00	0	0.00								
Water (kmol/h)	18.015	17,468		17,398		17,398									
TOTAL WET (kmol/h)		17,468		17,398		17,398									
			,684	313	3,429	313	3,429								
Molecular Weight	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \			18	3.0	18	8.0								
Notes :			Issue:	Α	Date	В	Date		Date		Date		Date		Page
			Description:	FOR S	STUDY	HEAT	DETAIL								4
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:										1		1

Table 4. Heat and Material Balance for Sour PSA Power Generation Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR28	300/P03	3/1001				
		ΝΛ	SC B	ALAN	ICE		Project No.	:	61LR2800		Plant:		SA POWE		
CONSULTANCY		IVI	133 B	ALAI	4CL		Client	:	AIR PROI	DUCTS	Location:	<b>EDMONT</b>	ON, ALBE	RTA	
The information contained herein is is issued on the understanding that							_								
JACOBS ENGINEERING UK LTD. 1							Case	:	4,472.5 to		-	gasificati	on		
contract.						1			for powe					1	
STREAM NUMBER		1	l		2		3		За		Bb		3c		3d
STREAM NAME		PETC FEEDS		GASIFICA OXYGE	TION UNIT		TION UNIT		REACTOR		EACTOR UENT		TO FEED NT EXCH		ROM FEED
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	0	0.00	0	0.00	7,026	34.13	7,026	34.13	14,962	52.42	14,962	52.42	14,962	52.42
Nitrogen	28.013	0	0.00	129	2.00	220	1.07	220	1.07	220	0.77	220	0.77	220	0.77
Carbon Monoxide	28.010	0	0.00	0	0.00	8,954	43.50	8,954	43.50	1,017	3.56	1,017	3.56	1,017	3.56
Carbon Dioxide	44.010	0	0.00	0	0.00	3,791	18.42	3,791	18.42	11,752	41.17	11,752	41.17	11,752	41.17
Methane	16.043	0	0.00	0	0.00	13	0.06	13	0.06	13	0.05	13	0.05	13	0.05
Argon	39.948	0	0.00	194	3.00	194	0.94	194	0.94	194	0.68	194	0.68	194	0.68
Hydrogen Sulphide	34.080	0	0.00	0	0.00	353	1.71	353	1.71	377	1.32	377	1.32	377	1.32
Carbonyl Sulphide	60.070	0	0.00	0	0.00	26	0.13	26	0.13	2	0.01	2	0.01	2	0.01
Ammonia	17.030	0	0.00	0	0.00	6	0.03	6	0.03	6	0.02	6	0.02	6	0.02
Oxygen	31.999	0	0.00	6,131	95.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Petcoke (tonnes/day)		4,472.5 (1)													
Temperature	°C	25		121		246		290		428		300		256	
Pressure	bara	1.00		83.34		67.86		67.56		67.16		66.56		66.26	
Total Dry Molar Flow (km		-	-	6,454	100.00	20,582	100.00	20,582	100.00	28,543	100.00	28,543	100.00	28,543	100.00
Water (kmol/h)	18.015	-		0		32,949		32,949		24,987		24,987		24,987	
TOTAL WET (kmol/h)		-		6,454		53,531		53,531		53,531		53,531		53,531	
Total Mass Flow (kg/h)	al Mass Flow (kg/h) 186,3			207	,550	1,05	3,201	1,05	3,201	1,05	3,201	1,05	3,201	1,05	3,201
Molecular Weight	107			32	2.2	19	9.7	19	9.7	19	9.7	1	9.7	19	9.7
Notes :				Α	Date	В	Date		Date		Date		Date		Page
Stated mass flow rep	resents dry	basis.	Description:	FOR	STUDY	HEAT	DETAIL								1
As received coke cor			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:											1	1

Table 4 cont'd. Heat and Material Balance for Sour PSA Power Generation Case

<b>JACOBS</b>	,	JACOBS	CONSU	JLTANC'	Y UK LTI	)	Document No.	:		800/P03	3/1001				
CONSULTANCY		MΔ	SS B	ΔΙ ΔΝ	JCF		Project No.	:	61LR280		Plant:		SA POWE		
							Client	:	AIR PRO	DUCTS	Location:	EDMONT	ON, ALBE	RTA	ļ
The information contained herein is is issued on the understanding that							0		4 472 E 4	nnoo/do	notooko	accificati	an .		
JACOBS ENGINEERING UK LTD. Toontract.	The data contain	ed in this docum	ent is subject to c	hange during the	design stage of ar	ny subsequent	Case	÷		onnes/day r producti	•	gasilicati	OII		
STREAM NUMBER		.9	ie		4		5		6		7		8		9
STREAM NAME		DESATI					GAS TO		N DILUENT		GAS TO		MBUSTOR		MBUSTOR
OTTE WITH WE			ED	SOUR P	SA FEED		BLOCK		ER BLOCK	SOUR CO			RT FUEL		D FUEL
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	14,962	52.42	14,949	52.64	14,029	91.40	0	0.00	920	7.05	0	0.00	920	6.77
Nitrogen	28.013	220	0.77	220	0.77	197	1.29	12,550	99.30	22	0.17	0	0.00	22	0.17
Carbon Monoxide	28.010	1,017	3.56	1,017	3.58	787	5.13	0	0.00	230	1.76	0	0.00	230	1.69
Carbon Dioxide	44.010	11,752	41.17	11,647	41.01	152	0.99	0	0.00	11,496	88.09	0	0.00	11,496	84.58
Methane	16.043	13	0.05	13	0.05	10	0.07	0	0.00	3	0.02	541	100.00	544	4.00
Argon	39.948	194	0.68	193	0.68	173	1.13	88	0.70	20	0.15	0	0.00	20	0.15
Hydrogen Sulphide	34.080	377	1.32	358	1.26	0	0.00	0	0.00	358	2.75	0	0.00	358	2.64
Carbonyl Sulphide	60.070	2	0.01	2	0.01	0	0.00	0	0.00	2	0.01	0	0.00	2	0.01
Ammonia	17.030	6	0.02	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Oxygen	31.999	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00
Petcoke (tonnes/day)															
Temperature	°C	245		48		35		15		44		25		44	
Pressure	bara	65.96		65.00		28.59		1.01		1.30		1.30		1.30	
Total Dry Molar Flow (km	nol/h, %)	28,543	100.00	28,399	100.00	15,348	100.00	12,638	100.00	13,051	100.00	541	100.00	13,591	100.00
Water (kmol/h)	18.015	24,987		58		1		0		14		0		14	
TOTAL WET (kmol/h)		53,531		28,457		15,349		12,638		13,064		541		13,605	
Total Mass Flow (kg/h)	al Mass Flow (kg/h) 1,0			598	,644	69,	628	355	5,104	528	,235	8,	679	536	5,914
Molecular Weight	, <b>,</b> ,			2′	1.0	4	.5	28	8.1	40	).4	1	6.0	3	9.5
Notes :				Α	Date	В	Date		Date		Date		Date		Page
			Description:	FOR S	STUDY	HEAT	DETAIL								2
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:		7 22 30		5 : <sub>4</sub> : 00							1	4
			Approved:										1		1

Table 4 cont'd. Heat and Material Balance for Sour PSA Power Generation Case

<b>JACOBS</b>		JACOBS	CONSU	JLTANC	Y UK LTI	)	Document No.	:	61LR2	300/P03	3/1001				'
		RA A	SS B	AI AN	ICE		Project No.	:	61LR2800	)	Plant:	SOUR PS	SA POWER	₹	
CONSULTANCY		IVI <i>F</i>	133 D	ALAI	NCE		Client	:	AIR PROI	DUCTS	Location:	<b>EDMONT</b>	ΓΟΝ, ALBE	RTA	
The information contained herein is is issued on the understanding that JACOBS ENGINEERING UK LTD. contract.	no part thereof s	shall be copied or	communicated to	a third party with	nout authorisation i	n writing from	Case	:	4,472.5 to		•	gasificati	ion		
STREAM NUMBER		1	0	,	11	1	2	1	13	1	14		15		
STREAM NAME			MBUSTOR N FEED		MBUSTOR E GAS		RIC ACID DUCT		BED FLUE AS	-	UENT TO R BLOCK	CO <sub>2</sub> TO	EXPORT		
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)		
Hydrogen	2.016	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Nitrogen	28.013	49	2.00	71	0.55	0	0.00	71	0.57	1	0.57	70	0.57		
Carbon Monoxide	28.010	0	0.00	1	0.01	0	0.00	1	0.01	0	0.01	1	0.01		
Carbon Dioxide	44.010	0	0.00	12,270	95.08	0	0.00	12,270	97.81	194	97.81	12,076	97.81		
Methane	16.043	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Argon	39.948	73	3.00	93	0.72	0	0.00	93	0.74	1	0.74	91	0.74		
Hydrogen Sulphide	34.080	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Carbonyl Sulphide	60.070	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Ammonia	17.030	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Oxygen	31.999	2,312	95.00	110	0.85	0	0.00	110	0.88	2	0.88	108	0.88		
Sulphur Dioxide	64.063	0	0.00	360	2.79	0	0.00	0	0.00	0	0.00	0	0.00		
Sulphuric Acid	98.078	0	0.00	0	0.00	360	100.00	0	0.00	0	0.00	0	0.00		
Petcoke (tonnes/day)															
Temperature	°C	25		200		30		30		30		30			
Pressure	bara	2.00		1.04		1.01		29.80		29.80		152.00			
Total Dry Molar Flow (kn	nol/h, %)	2,433	100.00	12,905	100.00	360	100.00	12,545	100.00	198	100.00	12,346	100.00		
Water (kmol/h)	18.015	0		2,380		0		33		0		0			
TOTAL WET (kmol/h)		2,433		15,284		360		12,578		198		12,346			
Total Mass Flow (kg/h)	,			615	5,163	35,	292	549	9,828	8,0	686	540	0,548		
Molecular Weight		32	2.2	40	0.2	98	3.1	43	3.7	43	3.8	4	3.8		
Notes :			Issue:	Α	Date	В	Date		Date		Date		Date		Page
			Description:	FOR S	STUDY	HEAT	DETAIL								3
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:												

Table 4 cont'd. Heat and Material Balance for Sour PSA Power Generation Case

JACOBS	,	JACOBS	CONSU	JLTANC	Y UK LT	)	Document No.	:		800/P03					
		М	SS B	AI AN			Project No.	:	61LR280	-	Plant:	SOUR P	SA POWER	3	
CONSULTANCY		IVI	133 D	ALAI	1CL		Client	:	AIR PRO	DUCTS	Location:	EDMON	TON, ALBE	RTA	
The information contained herein is is issued on the understanding that I JACOBS ENGINEERING UK LTD. 1 contract.	no part thereof s	hall be copied or	communicated to	a third party with	out authorisation i	n writing from	Case	:		onnes/day r product	petcoke	gasificat	ion		
STREAM NUMBER		1	6	1	17	1	8		19	2	20		21		
STREAM NAME			MBUSTOR BFW		MBUSTOR TEAM		RXR HP EAM		. SUPER HP STEAM		MBUSTOR TEAM		EATED LP EAM		
COMPONENT	MW	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)	kmol/h	mol% (dry)
Hydrogen	2.016	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Nitrogen	28.013	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Carbon Monoxide	28.010	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Carbon Dioxide	44.010	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Methane	16.043	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Argon	39.948	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Hydrogen Sulphide	34.080	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Carbonyl Sulphide	60.070	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Ammonia	17.030	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Oxygen	31.999	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Sulphur Dioxide	64.063	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Sulphuric Acid	98.078	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Petcoke (tonnes/day)															
Temperature	°C	30		286		286		513		160		232			
Pressure	bara	75.00		70.00		70.00		70.00		6.00		5.50			
Total Dry Molar Flow (km	nol/h, %)	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00		
Water (kmol/h)	18.015	10,990		10,551		8,593		19,144		17,681		17,681			
TOTAL WET (kmol/h)		10,990		10,551		8,593		19,144		17,681		17,681			
Total Mass Flow (kg/h)	tal Mass Flow (kg/h)			190	,071	154	,814	344	1,885	318	,527	318	3,527		
Molecular Weight		18	3.0	18	3.0	18	3.0	18	8.0	18	3.0	1	8.0		
Notes :			Issue:	Α	Date	В	Date		Date		Date		Date		Page
			Description:	FOR S	STUDY	HEAT	DETAIL								4
			Made By:	ARA	29-Jan-09	LEW	16-Apr-09								of
			Checked:												4
			Approved:												7

# Appendix 4.

# **Risk Register**

Air Pı	roducts CO2 Capture To	echnolog	jy Risk F	Register					
Risk No.	Risk Name	Event Occ this will be for "runnin		bability that target date 1 Jan 2020,	Event Valu	ue: Delta P (\$MM)	roject NPV	Event <b>Probability</b> Input Data.	Brief Summary of Session Notes: Event Valuation and other Impact Details (See Session Notes for additional detail)
		low	average	high	low	average	high		
4	More aggressive than planned corrosion in vessels (particularly reaction system and piping)	70.00%	81.88%	95.00%	(\$0.9)	(\$9.5)	(\$67.0)	.7 to .9 0.75 .9 to .95 0.8	See calculations page and session notes.
2	PSA recovery (R) is lower than predicted	10.00%	18.75%	25.00%		(\$3.9)		0.2 0.15 0.25 0.1 to .2	Distinct P of a 1% drop in R, lasting for 12 months. Loss \$ = 1% of scfs from H2. OR Loss = 1% of power (may be less fo an issue for power than H2 case.) Use \$3/1000 scfs for H2.  (\$3MM/annum)
1	PSA Adsorbent dies faster than originally planned changeout schedule (10 year basis)	40.00%	51.67%	70.00%	(\$1.4)	(\$2.7)	(\$4.6)	0.5 .4 to .7 .4 to .6	Replacment at 6 years vs 10. (Worst case forever = 5%.) (Best case would eventually fix.) Cost for reload = for 4 trains = B

Air Pr	oducts CO2 Capture Te	chnolog	y Risk F	Register					
Risk No.	Risk Name	Event Occ this will be a for "running		bability that target date n Jan 2020,	Event Valu	ıe: Delta Pı (\$MM)	roject NPV	Event <b>Probability</b> Input Data.	Brief Summary of Session Notes: Event Valuation and other Impact Details (See Session Notes for additional detail)
		low	average	high	low	average	high		
6a	Variability in feedstock composition beyond	10.00%	15.00%	20.00%		(\$7.7)		.1 to .2	Impact 1 = Higher S, beyond the design range. Result: Would have to cycle the PSA faster . Recovery would drop, less than 1%. // Duration = 3 to 6 months. USe \$3MM/annum value
	expectations								estimated for Risk 2. // 6a to 6b Correlation: If 2 yes, 1 yes. If 1 yes, 2 may not happen to same degree. Use H2 mode as the risk analysis mode.
6b	Variability in feedstock composition beyond	5.00%	7.50%	10.00%		(\$76.6)		.05 to .1	Impact 2 = Higher S results in backoff on throughput to combuster. (Too many Btus to combuster). More sensitive to H2 case than power case. / For H2 case: Assume 10% throughput
	expectations								loss for 50% more S in feed. Duration = 3 to 6 months. (Sales rev for H2 = \$300MM/year, so assume \$30 MM per year rev loss
									during period of higher S.) Use H2 mode as the Risk analysis mode.
12	More support fuel required in	1.00%	5.25%	10.00%	(\$12.2)	(\$16.3)	(\$24.5)	.01 to.05	
	More support fuel required in oxycombustor							05 to 4	Assume \$150k/day Opex Debit. (assume \$7/MM Btu nat gas) Duration = 6 months, or less, until you find a home for H2 or change feedstock.
								.05 to .1	

Air Pr	oducts CO2 Capture Te	chnolog	y Risk F	Register					
Risk No.	Risk Name	Event Occ this will be a for "running		bability that target date Jan 2020,	Event Valu	ue: Delta Pi (\$MM)	roject NPV	Event <b>Probability</b> Input Data.	Brief Summary of Session Notes: Event Valuation and other Impact Details (See Session Notes for additional detail)
		low	average	high	low	average	high		
13	Acid reactions do not occur as predicted, incomplete conversion of SO2 into sulfuric acid	40.00%	45.00%	50.00%	(\$6.8)	(\$17.0)	(\$34.1)	.4 to .5	SO2 slips back to CO2 product. // SO2 in regen gas. // Need something on regen gas to clean it up. // Emissions issue // e.g., design for 10 ppm SO2 getting through and now we get 20 to 40 ppm through. // Would have to regen TSA at higher f. // 1 to 5 \$MM/ year. // Duration = ?  Might let it go at this low cost Might not be an easy fix.
8	Mechanical issues caused by corrosion in PSA								
	Covered in 4 as worst case situation.								
10	Excessive capital requirements for acid section	0.50%	0.75%	1.00%	(\$7.1)	(\$81.4)	(\$155.7)	"very very low" <0.01	
15	CO2 spec is not met	30.00%	35.00%	40.00%		(\$123.9)		.3 to .4	Having problems getting rid of CO2. Remedy = "Quick" insert of inert removal system. / C++ Capex / Could lose 6 months of operation due
									to inability to emit CO2 due to regs, OR it could be vented and pay penalty or buy CO2 dredits.  Could be bi-modal
									More probable for power case.

Air Pr	oducts CO2 Capture Te	echnolog	y Risk F	Register					
Risk No.	Risk Name	Event Occ this will be a for "running		bability that target date n Jan 2020,	Event Valu	ue: Delta Pi (\$MM)	roject NPV	Event <b>Probability</b> Input Data.	Brief Summary of Session Notes: Event Valuation and other Impact Details (See Session Notes for additional detail)
		low	average	high	low	average	high		
16	CO2 Regulatory specs end up to be tighter than design (expectation) [Assume this is a spec in place that is changed.]		10.00%		(\$32.5)	(\$50.7)	(\$68.9)	0.1	Project would shift into future
17	Extra downtime due to solving problems with heavy metals	30.00%	35.00%	40.00%	(\$68.8)	(\$103.1)	(\$137.5)	.3 to .4	Solution = capex for guard bed. (Capex = B.) Assume 6 month downtime (margin loss).
34	Development time extended due to change in feedstock		5.00%		(\$39.4)	(\$98.8)	(\$158.2)	0.05	6 to 18 months Lost time. (back to demo plant and design tweak)
39	Long-term liability cost due to landspread		2.00%			(\$178.6)		0.02	Very high potential cost (E)

## Appendix 5.

# **Primary Cases—HAZID**

HAZARD IDENTIFICATION - Basic Flowscheme: Register					
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items
Sour PSA					Particulates affecting performance? Water dropping out?
	Novel Operating Pressure	Pressure is higher than SMR operations we are used to. Mechanical issues, pressure vessel design. Does historical valve information apply? Valve integrity in long term (handle some level of dust) and short term. Yield, performance, on-stream factor.			Valve effects on process performance
	Leak to environment		Yes	Valves will be spec'd for conditions. Double block, bleed to FI with alarm	
	Leak to tailgas	Too much syngas going to combustor (above rating of combustor)	Yes	Valves will be spec'd for conditions. Instrumentation & bypass	
	Potential for liquid H2O formation in PSA vessels	Corrosion issues with liquid water and acid gas leading to acid formation and decreased adsorbent integrity. Low temperature (25F) at coldest point of cycle.	Yes	Design PSA for substantial free water & minimize liquid water carryover from upstream (demister, heat trace piping). Add inert gas	Heat trace piping leading to PSA. Design for substantial H2O into PSA unit.
	Vessel leak/rupture due to cyclic fatigue or corrosion		Yes	Rigorous Mech Eng: Design metallurgy for cyclic process & calculate vessel life. Adjust cycle time. Vessel inspections.	
	Presence of H2S	H2 embrittlement	Yes	Material selection.	Look into. Test data?
	Particulates lead to valve failure	Particulates carrying over from carbon guard beds	Yes	SOP will be to replace valve if dusting occurs	

Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items
ower					
	H2S levels beyond design spec in H2	Feed composition changes or control issue (large step change increase in H2S). Emission issues coming out of power block. Corrosion issues.	Yes	Feed-forward control and analyzers to adjust cycle time.	
	Adsorbent exposure while unloading	Health risks from Hg, arsenic, etc	Yes	Rigorously follow SOP, including PPE. Use specialty contractors.	
	Adsorbent disposal issues	See earlier information on used adsorbent.	Yes		
	H2 leak	Assumed ignition source	Yes	Good design, SOP, inspection, metallurgy choice	
	Cold weather & pressure & chemicals effect on valve integrity		Yes	Experience, good design, testing in demo plant in the area	
	Pressure relief situation will release sour gas	Likely will go to sour flare	Yes	Industry standard sour flare	
urge Tank	k Between Sour PSA an	d Oxycombustor			

HAZARD	HAZARD IDENTIFICATION - Basic Flowscheme : Register						
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items		
Oxycombu	Oxycombustor						
	Corrosion of coils	SOx, NOx. Leads to HP steam into vessel "Burp."	Yes	Flapper type of safety valve. Low set pressure. Materials of construction of coils. Inspection.			
	Corrosion of refractory & fouling of downstream surfaces		Yes	Periodic maintenance & choice of refractory. Sensors/paint.			
	Overpressure & "vessel" rupture	Corrosion, coil rupture from HP steam, downstream blockage	Yes	Flapper type of safety valve. Pressure sensors on upstream valves.			
	Particulate blockage in burner (particles from PSA)	Debris buildup on nozzles. Carbon combustion?	Yes	Bend in line & dropout & inspection. Thermocouples.			
	Lose flow to steam coils but still burning	Also possible in startup before steam generation is fully up elsewhere in unit	Yes	Interlock			
	Erosion of burner tips	From carrying forward particles from PSA adsorbent	Yes	See particulate blockage.			
	Loss of O2 flow		Yes	Interlock			
	Loss of flame with continued flow of fuel and O2		Yes	Secondary burner. Interlock linked to flame detector.			
	Corrosion on BFW coil	From liquid dropout. Need to maintain temperature above dewpoint.	Yes	Temperature monitoring. Materials of construction.			
	Poly-T-Acid Formation	O2, H2O, and S. Need to avoid dewpoint since we have all the compounds.	Yes	Temperature monitoring. Materials of construction. Increase margin above dewpoint of outlet temperature (200°C minimum?)			

HAZARD IDENTIFICATION - Basic Flowscheme: Register						
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items	
Flue Gas Cooler/ Condenser						
	High temperature to compressor	Loss of cooling water (or air or glycol for Alberta)	Yes	Flow & temp sensors linked to compressor	Talk to Mike Wilcox about compressor tolerance	
	Acid corrosion		Yes	Materials of Construction. Design for HCl.		
	Fouling in bed or on exchanger	From particulates. Contact cooler.	Yes	ΔP Monitor, ΔT Monitor.		
Compresso	or					
	Low P at Compressor Suction	Due to $\Delta P$ buildup from depositing solids.				
	High temperature to compressor	Loss of cooling water (or air or glycol for Alberta) or loss of interstage cooling	Yes	Flow & temp sensors linked to compressor to trip system	Talk to Mike Wilcox about compressor tolerance	
	Liquid to compressor resulting in sudden failure		Yes	Superheat the upstream heater and knockout		
	Loss of containment in KO system or downstream lines		Yes	pH monitor in downstream lines & inspection.		

AZARD	DIDENTIFICATION	- Basic Flowscheme : Register			
Flow- cheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items
)2 Comp	pression				
	2 phase flow in final compression stage	From CO2 impurities	Yes	Proper design. Monitor CO2 purity & Temperature	
	High temperature to compressor	Loss of cooling water (or air or glycol for Alberta)	Yes	Flow & temp sensors linked to compressor to trip system	
	Acid carryover to compressor	At shutdown	Yes	SOP, purges	
	Loss of containment with high pressure acid due to corrosion		Yes	Material selection, good design, pilot/demo plant data, lined vessel	
			Yes		
	high pressure acid due to bad seals		Yes	Lined Vessels	
	Loss of containment with high pressure acid due to unexpected reactions	e.g. Cls in makeup H2O or other salts	Yes	Lined Vessels. Specification of makeup water & constant analysis	
	arroxpootod rodotiono				
	Flash of dissolved gases on depressurization		Yes	Design	
	Flash of dissolved gases on	Tube rupture	Yes	Design pH sensor	
	Flash of dissolved gases on depressurization  Contamination of cooling	Tube rupture  Acid mist carryover		•	

HAZARD IDENTIFICATION - Basic Flowscheme : Register						
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items	
Dehydratio	<b>Dehydration</b> Note, Regen gas not known at this time					
	Adsorbent degradation		Yes	Will do life testing		
	Hot regen gases causing corrosion		Yes	Design		
Cold Box						
	Water breakthrough	Acids to cold box. Corrosion & blockage	Yes	Demo plant testing		
	Acids to cold box	If TSA not working properly	Yes	Probes prior to cold box		
	Hg compound deposition issues		Yes	Hg bed upstream of cold box		
	CO2 hydrates formation		Yes	Modeling calculations		

HAZARD IDENTIFICATION - Basic Flowscheme: Register						
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items	
Power Production						
	Carbonyls decomposing in expander		?		Models, calcs, chemistry, Gibbs free energy calcs	
	Dust particles from PSA going to expander		Yes	Filter if necessary		
Steam Generation						
Novel Flue gas	s on HX Surfaces					
	Corrosion in HRSG	High sulfur	Yes	Monitor product gas from PSA (design spec on H2S)		

# Appendix 6.

## **Alternative Cases—HAZID**

#### Alternate Flowschemes HAZID Part 1

HAZARD IDENTIFICATION - Alternate Flowscheme C					
Oxy-combustor heat recovery and economizer condenser					
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items
Conventional economizer coil limited to flue gas temperatures of 320-350°F					
Uses standal	one condensing economize	er with upgraded metallurgy for additional heat recovery			
	Cavitation resulting from greater potential for unexpected 2-phase flow	Areas of condensation where 2-phase flow is not expected.	Yes	Instrumentation controls on temperature around exchangers.	
	Steam breakthrough into exchanger	Tube rupture in condensing economizer. Greater risk with 70 bar steam vs 5 bar CW. BFW will flash to steam into flue gas and water will flow into the process side.	Yes	Design tubes for high pressure and condensing acid service.	
	Steam flowing into combustor	As a result of tube rupture and overpressure in condensor.	Yes	Flapper safety valve on oxycombustor.	

#### **Alternate Flowschemes HAZID Part 2**

HAZARD IDENTIFICATION - Alternate Flowscheme B						
Oxy-combustor heat recovery and economizer condenser						
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items	
Neutralize Acids and Landspread/ Landfill						
	Introduction of new, potentially toxic, corrosive substances	Neutralization chemicals & products: ammonia, ash from power station, basic substances, caustic solution, other materials? Heavy metals in landfill material (depends on composition of petcoke)	Yes?	Industry standard precautions for handling. Send to hazardous waste landfill.		
	Unknown, unexpected byproducts of neutralization reactions		Yes	Calculations. Demo/pilot plant data. DOE work will support.		
	Exposure to solids	Between pond and landfill (toxic material with heavy metals)	Yes	SOPs. Heavy metal removal upstream		
	Heat generation from neutralization	Heat may build up if neutralization is done in tank	Yes	Design issue. Control systems. Previous work will dictate.		
	Solids formation in unwanted location	If neutralization is done in situ. Plugs up absorber. Solids are dissolved in water and collect at the bottom.		Design issue. Monitor and add diluent water as necessary.		
	Pond overflow	Contamination of environment	Yes	SOPs and design considerations.		
	Volatile vapors from pond		Yes	DOE work & demo plant will support.		
	For landspread case, unknowns or unexpected leach issues cause problems	Liability and cost risk as well. Long term uncertainty.	Yes	Constant monitoring to ensure adequate disposal choice. Or send all to lined hazardous landfill.		
	Transport of caustic		Yes	Standard SOP and equipment. Alternate chemicals		
	Storage of caustic		Yes	Standard SOP and equipment. Alternate chemicals		

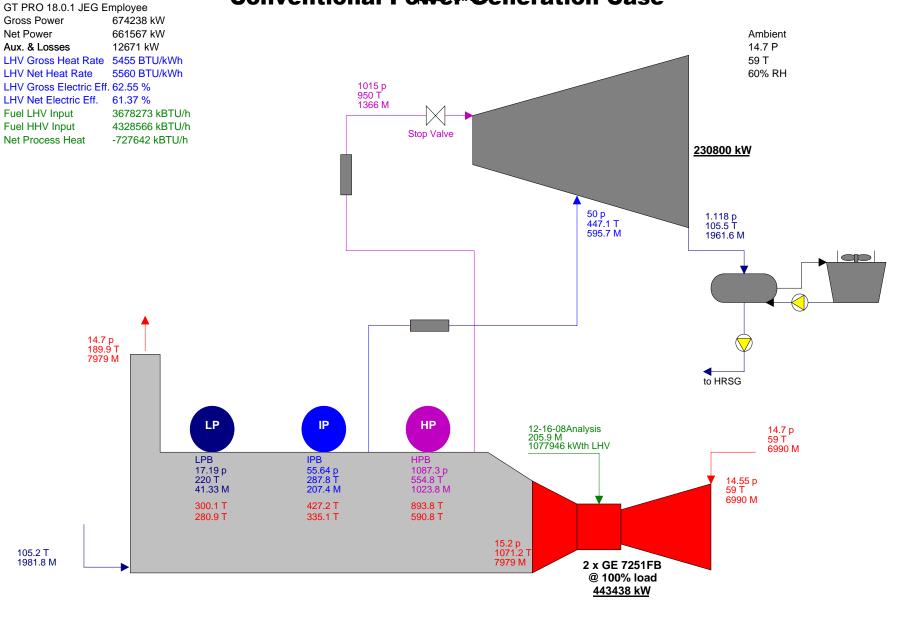
#### **Alternate Flowschemes HAZID Part 3**

HAZARD IDENTIFICATION - Alternate Flowscheme B							
Oxy-combustor heat recovery and economizer condenser							
Flow- scheme	Name of Hazard	Notes/Comments	HAZARD Mitigable/ Manageable?	How?	Action Items		
Neutralize Aci	Neutralize Acids and Landspread/ Landfill						
	Eliminated risks from	n the Acid Formation & Separation System:					
	No transport of acid No storage of acid No flash issue upon lowering pressure of acid streams	Possible. Depends on method of acid neutralization.					

## Appendix 7.

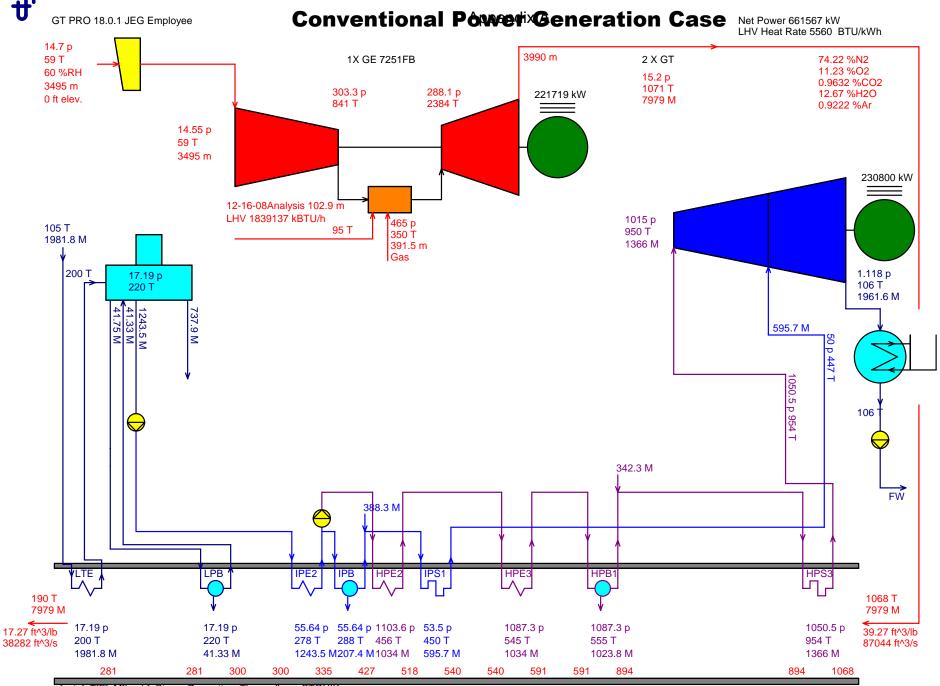
## **Power Block Simulation Results**

## Conventional Power Generation Case



p [psia] T [F] M [kpph], Steam Properties: Thermoflow - STQUIK

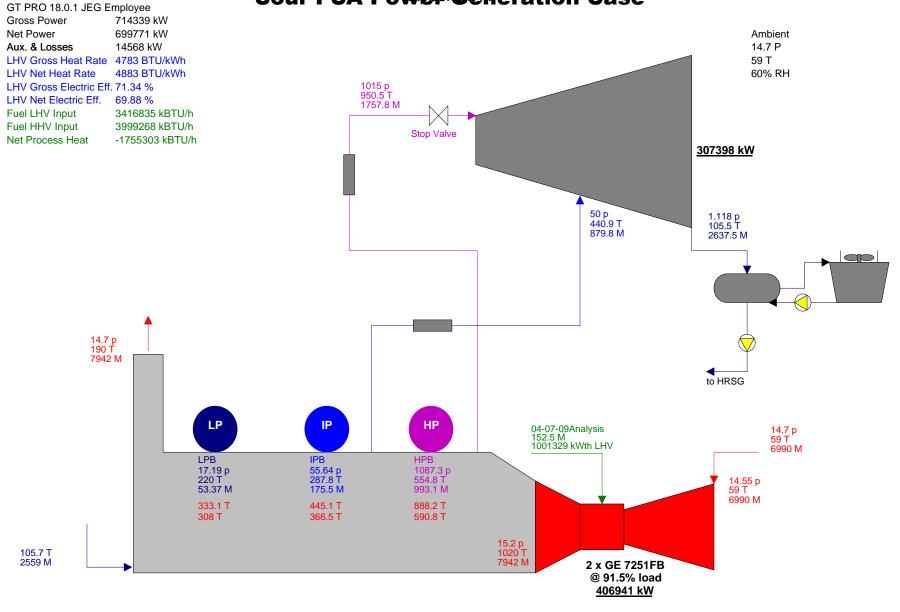
284 01-27-2009 15:27:44 file=M:\2 Calcs\Power Block\2009-01-27 2x1 7FB 1000#50# HotAdm 2000C SCR.GTP



p[psia], T[F], M[kpph], Steam Properties: Thermoflow - STQUIK

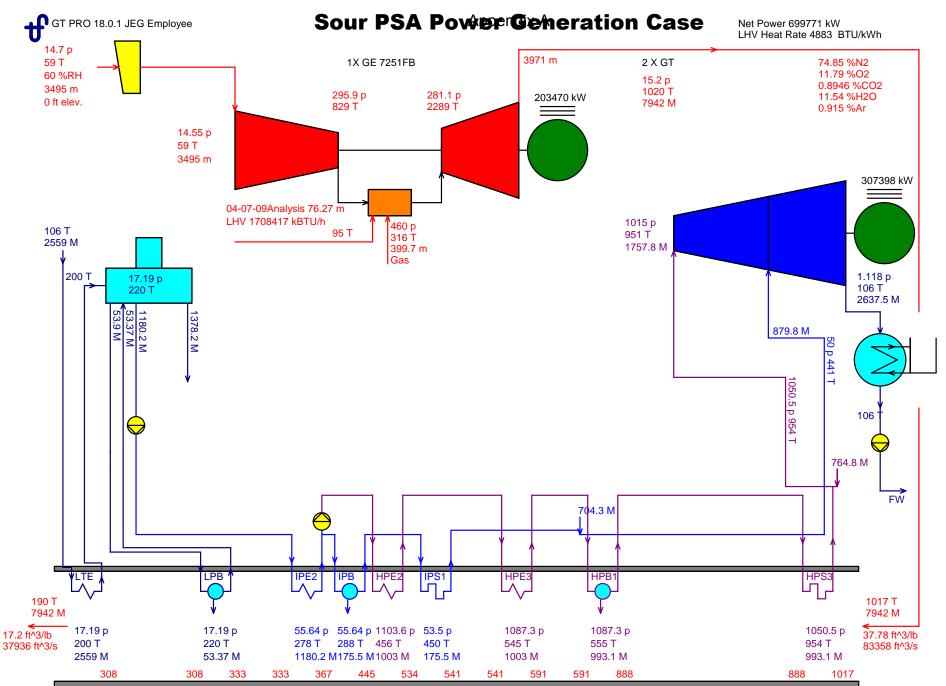
284 01-27-2009 15:27:44 file=M:\2 Calcs\Power Block\2009-01-27 2x1 7FB 1000#50# HotAdm 2000C SCR.GTP

#### Sour PSA Power Generation Case



p [psia] T [F] M [kpph], Steam Properties: Thermoflow - STQUIK

284 04-13-2009 15:40:24 file=M:\2 Calcs\Power Block\2009-04-13 2x1 7FB 1000#50# HotAdm 2000C SCR AP Fuel.GTP



p[psia], T[F], M[kpph], Steam Properties: Thermoflow - STQUIK

284 04-13-2009 15:40:24 file=M:\2 Calcs\Power Block\2009-04-13 2x1 7FB 1000#50# HotAdm 2000C SCR AP Fuel.GTP

# JACOBS Consultancy

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Member, Jacobs Engineering Group

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# **Appendix B**





#### **Gas Analysis Report**

Air Products and Chemicals 7201 Hamilton Boulevard Allentown, PA 18195

610-481-3998;

Attn.: Mr. Jeffrey Hufton; E-mail: Huftonjr@airproducts.com

Sample ID: Mix Gas Sample A Comments: 1 of 2 Samples received in 500 cc customer Cylinder.

AAL Number: 9683-1 Received On: 12-Feb-09 Report Date: 20-Feb-09 PO Number: credit card

Sample Date: --Sample Time: --

Docult

	Res	<u>sult</u>
Non-Condensable Gases		
	5.82	0.01
	nd	0.01
	54.6	0.05
	3.80	0.05
	32.8	0.05
	0.01	0.05
	2.86	0.01
		0.001
	<u>% v/v</u>	<u>D.L.</u>
	0.002	0.001
	0.025	0.001
	nd	0.001
	0.02	0.001
	Gases	Gases         % v/v           5.82         nd           54.6         3.80           32.8         0.01           2.86            % v/v         0.002           0.025         nd           nd         nd

**Comments:** Peak ID based upon  $t_{\Gamma}$  match against target analyte standards. **D.L.** = report detection limit.  $\mathbf{nd}$  = indicates the concentration is less than the report detection limit.  $\mathbf{--}$  = test not performed. **L.T.** = less than the amount specified. % = percent.  $\mathbf{ppm}$  = parts per million.  $\mathbf{ppb}$  = parts per billion.  $\mathbf{v/v}$  = volume analyte/volume sample.  $\mathbf{w/w}$  = weight analyte/weight sample.

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AAL Number: 9683-1

#### Gas Mix Sample A

#### GC/MS C6+ Extended Range Results

Libr. Hit List <sup>1</sup> &/or <u>Target Analyte(s)</u>	Result <u>% v/v</u>
Aliphatic Hydrocarbons (C <sub>6</sub> range):	 nd 0.001
Aliphatic Hydrocarbons ( $C_7$ range):	 nd 0.001
Aliphatic Hydrocarbons (C <sub>8</sub> range):	 nd 0.001
Aliphatic Hydrocarbons (C9 range):	 nd 0.001
Aliphatic Hydrocarbons (C10 range):	 nd 0.001
Aliphatic Hydrocarbons ( $C_{11} - C_{14}$ range):	 nd 0.001

Aromatic Hydrocarbons:	Peak ID/Scan No.	Result ppm v/v
Benzene	a/573	187
Toluene	a/884	5.9
Ethylbenzene	a/1154	0.5
m+p Xylenes	a/1175	0.4
o-Xylene	a/1240	0.2
Naphthalene	a/1936	1.9

Peak ID. Category:  $\bf a$  = computer library match >900, + retention time ( $\bf t_r$ ) match with a calibration std.  $\bf b1$  = computer library match >900,  $\bf not$  confirmed by a calibration std.  $\bf b2$  = Computer library match between 800 - 900, not confirmed by a ( $\bf t_r$ ) match with a calibration std.  $\bf c$  = Computer library match <800, potential structure + functional group information only.

Comments: Peak ID based upon t<sub>r</sub> match against target analyte standards. D.L. = report detection limit. nd = indicates the concentration is less than the report detection limit. -- = test not performed. L.T. = less than the amount specified. % = percent. ppm = parts per million. ppb = parts per billion. v/v = volume analyte/volume sample. w/w = weight analyte/weight sample.



A T L A N T I C A N A L Y T I C A L L A B O R A T O R Y

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ID: Air Products and Chemicals

AAL Number: 9683-1

#### Gas Mix Sample A

Volatile Sulfur Compound	ds (VSC, ppm v/v)	Result	<u>D.L.</u>
Hydrogen Sulfide (H <sub>2</sub> S): Carbonyl Sulfide (COS):		21,580 374	0.1 0.1
Sulfur Dioxide (SO <sub>2</sub> ):		nd	0.1
Methyl Mercaptan:		4.8	0.1
Ethyl Mercaptan:		6.9	0.1
Dimethyl Sulfide:		nd	0.1
Carbon Disulfide:		nd	0.1
Isopropyl Mercaptan		nd	0.1
t-Butyl Mercaptan:		nd	0.1
n-Propyl Mercaptan:		nd	0.1
Methyl Ethyl Sulfide:		nd	0.1
sec-Butyl Mercaptan:		nd	0.1
Thiophene:		2.6	0.1
Isobutyl Mercaptan:		nd	0.1
Diethyl Sulfide:		nd	0.1
n-Butyl Mercaptan:		nd	0.1
Dimethyl Disulfide:		nd	0.1
3-Methylthiophene:		nd	0.1
Tetrahydrothiophene:		nd	0.1
2-Ethylthiophene:		nd	0.1
2,5-Dimethylthiophene:		nd	0.1
Diethyl Disulfide:		nd	0.1
Unknown Compounds:		nd .	0.1

Comments: Total Sulfur = 21,968 ppm v/v (2.20% v/v).

**D.L.** = report detection limit.  $\mathbf{nd}$  = indicates the concentration is less than the report detection limit.  $\mathbf{--}$  = test not performed. **L.T.** = less than the amount specified. % = percent.  $\mathbf{ppm}$  = parts per million.  $\mathbf{ppb}$  = parts per billion.  $\mathbf{v/v}$  = volume analyte/volume sample.  $\mathbf{w/w}$  = weight analyte/weight sample. **Unit Conversions:** 1 ppm v/v = 1 $\mu$ L/L = 1,000 ppb = 0.0001% v/v.

Reviewed By,

Richard F. Frisch

Addendum: - Chromatograms on-file Notebook data on-file



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page 3 of 3







#### **Gas Analysis Report**

Air Products and Chemicals AAL Number: 13566-1 7201 Hamilton Boulevard Received On: 24 Feb 10 Report Date: 18 Mar 10 PO Number: credit card Allentown, PA 18195 610-481-3998;

Attn.: Mr. Jeffrey Hufton; E-mail: Huftonjr@airproducts.com

Sample ID: Sour Syngas; 21435-60-1 Sample Date: --

Comments: 1 of 2 Samples received in 500 cc customer cylinder. Sample Time: --

		<u>Result</u>	
Non-Condensable	<u>: Gases</u>	% v/v	D.L.
Nitrogen:		28.5	0.01
Oxygen:		nd	0.01
Carbon Dioxide:		29.0	0.05
Carbon Monoxide:		0.61	0.05
Hydrogen:	***************************************	41.7	0.05
Argon:		0.10	0.05
Methane:	***************************************	0.17	0.01
Water Vapor:			0.001
<u>Hydrocarbons</u>		<u>% v/v</u>	<u>D.L.</u>
Ethylene:		nd	0.001
Ethane:		0.001	0.001
Propylene:		nd	0.001
Propane:		nd	0.001
Isobutane:		nd	0.001
n-Butane:		nd	0.001
Butene:		nd	0.001
Isopentane:		nd	0.001
n-Pentane:		nd	0.001
Pentenes:		nd	0.001
Hexanes+:		nd	0.001

**Comments:** Peak ID based upon  $t_r$  match against target analyte standards. **D.L.** = report detection limit.  $n\mathbf{d}$  = indicates the concentration is less than the report detection limit. -- = test not performed. **L.T.** = less than the amount specified. % = percent. ppm = parts per million. ppb = parts per billion. v/v = volume analyte/volume sample. w/w = weight analyte/weight sample.

Page 1 of 3



AAL Number: 13566-1

#### 21435-60-1

#### GC/MS C6+ Extended Range Results

Libr. Hit List <sup>1</sup> &/or <u>Target Analyte(s)</u>	Result % v/v
Aliphatic Hydrocarbons (C <sub>6</sub> range):	 nd 0.001
Aliphatic Hydrocarbons (C <sub>7</sub> range):	 nd 0.001
Aliphatic Hydrocarbons (C <sub>8</sub> range):	 nd 0.001
Aliphatic Hydrocarbons (C9 range):	 nd 0.001
Aliphatic Hydrocarbons (C10 range):	 nd 0.001
Aliphatic Hydrocarbons ( $C_{11} - C_{14}$ range):	 nd 0.001

Aromatic Hydrocarbons:	Peak ID/Scan No.	Result ppm v/v
Benzene	a/655	0.2
Toluene	/912	nd 0.1
Ethylbenzene	/1159	nd 0.1
m+p Xylenes	/1172	nd 0.1
o-Xylene	/1250	nd 0.1
Naphthalene	/1946	nd 0.1
Carbonyls:		
Nickel tertacarbonyl	/	nd 5 ppm
Iron pentacarbonyl	/	nd 1 ppm

Peak ID. Category: a = computer | ibrary match > 900, + retention time  $(t_f)$  match with a calibration std. b1 = computer | ibrary match > 900, not confirmed by a calibration std. b2 = computer | ibrary match | between 800 - 900, not confirmed by a  $(t_f)$  match with a calibration std. c = computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, potential structure + functional group information computer | ibrary match < 800, computer | ibrary mat

Comments: Peak ID based upon t<sub>r</sub> match against target analyte standards. D.L. = report detection limit. nd = indicates the concentration is less than the report detection limit. -- = test not performed. L.T. = less than the amount specified. % = percent. ppm = parts per million. ppb = parts per billion. v/v = volume analyte/volume sample. w/w = weight analyte/weight sample.





ID: Air Products and Chemicals AAL Number: 13566-1

#### 21435-60-1

Volatile Sulfur Compounds (VSC, ppm v/v)		Result	<u>D.L.</u>	
Hydrogen Sulfide (H <sub>2</sub> S):		10,550	0.1	
Carbonyl Sulfide (COS):		15	0.1	
Sulfur Dioxide (SO <sub>2</sub> ):		nd	0.1	
Methyl Mercaptan:		1.5	0.1	
Ethyl Mercaptan:		nd	0.1	
Dimethyl Sulfide:		nd	0.1	
Carbon Disulfide:		nd	0.1	
Isopropyl Mercaptan		nd	0.1	
t-Butyl Mercaptan:		nd	0.1	
n-Propyl Mercaptan:		nd	0.1	
Methyl Ethyl Sulfide:		nd	0.1	
sec-Butyl Mercaptan:		nd	0.1	
Thiophene:		nd	0.1	
Isobutyl Mercaptan:		nd	0.1	
Diethyl Sulfide:		nd	0.1	
n-Butyl Mercaptan:		nd	0.1	
Dimethyl Disulfide:		nd	0.1	
3-Methylthiophene:		nd	0.1	
Tetrahydrothiophene:		nd	0.1	
2-Ethylthiophene:		nd	0.1	
2,5-Dimethylthiophene:		nd	0.1	
Diethyl Disulfide:		nd	0.1	
Unknown Compounds:		nd	0.1	

Comments: Total Sulfur = 10,566 ppm v/v (1.06 % v/v).

D.L. = report detection limit. nd = indicates the concentration is less than the report detection limit. -- = test not performed. **L.T.** = less than the amount specified. % = percent. **ppm** = parts per million. **ppb** = parts per bllion.  $\mathbf{v/v}$  = volume analyte/volume sample.  $\mathbf{w/w}$  = weight analyte/weight sample. **Unit Conversions:** 1 ppm v/v = 1 $\mu$ L/L = 1,000 ppb = 0.0001% v/v.

Reviewed By,

Richard F. Frisch

Addendum: - Chromatograms on-file Notebook data on-file



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#### **Gas Analysis Report**

Air Products and Chemicals
7201 Hamilton Boulevard
Allentown, PA 18195
610-481-3998;
AAL Number: 13566-2
Received On: 24 Feb 10
Report Date: 18 Mar 10
credit card

Attn.: Mr. Jeffrey Hufton; E-mail: Huftonjr@airproducts.com

Sample ID: Sour Syngas; 21435-60-2 Sample Date: -- Comments: 2 of 2 Samples received in 500 cc customer cylinder. Sample Time: --

		Result	
Non-Condensable	Gases	% v/v	D.L.
Nitrogen:		38.6	0.01
Oxygen:		nd	0.01
Carbon Dioxide:		0.18	0.05
Carbon Monoxide:		0.69	0.05
Hydrogen:		60.3	0.05
Argon:		0.13	0.05
Methane:		0.12	0.01
Water Vapor:			0.001
Hydrocarbons		<u>% v/v</u>	<u>D.L.</u>
Ethylene:		nd	0.001
Ethane:		nd	0.001
Propylene:		nd	0.001
Propane:		nd	0.001
Isobutane:		nd	0.001
n-Butane:		nd	0.001
Butene:		nd	0.001
Isopentane:	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	nd	0.001
n-Pentane:		nd	0.001
Pentenes:		nd	0.001
Hexanes+:		nd	0.001

**Comments:** Peak ID based upon  $t_r$  match against target analyte standards. **D.L.** = report detection limit. **nd** = indicates the concentration is less than the report detection limit. -- = test not performed. **L.T.** = less than the amount specified. % = percent. **ppm** = parts per million. **ppb** = parts per billion. **v/v** = volume analyte/volume sample. **w/w** = weight analyte/weight sample.

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AAL Number: 13566-2

#### 21435-60-2

#### GC/MS C6+ Extended Range Results

Libr. Hit List <sup>1</sup> &/or Target Analyte(s)	Result % v/v
Aliphatic Hydrocarbons (C <sub>6</sub> range):	 nd 0.001
Aliphatic Hydrocarbons ( $C_7$ range):	 nd 0.001
Aliphatic Hydrocarbons (C <sub>8</sub> range):	 nd 0.001
Aliphatic Hydrocarbons (C9 range):	 nd 0.001
Aliphatic Hydrocarbons (C10 range):	 nd 0.001
Aliphatic Hydrocarbons ( $C_{11} - C_{14}$ range):	 nd 0.001

Aromatic Hydrocarbons:	Peak ID/Scan No.	Result <u>ppm v/v</u>
Benzene	/655	nd 0.1
Toluene	/912	nd 0.1
Ethylbenzene	/1159	nd 0.1
m+p Xylenes	/1172	nd 0.1
o-Xylene	/1250	nd 0.1
Naphthalene	/1946	nd 0.1
Carbonyls:		
Nickel tertacarbonyl	/	nd 5 ppm
Iron pentacarbonyl	/	nd 1 ppm

**Peak ID. Category:** a = computer library match >900, + retention time  $(t_r)$  match with a calibration std. **b1** = computer library match >900, not confirmed by a calibration std. **b2** = Computer library match between 800 - 900, not confirmed by a  $(t_r)$  match with a calibration std. **c** = Computer library match <800, potential structure + functional group information not

Comments: Peak ID based upon  $t_{\Gamma}$  match against target analyte standards. D.L. = report detection limit. nd = indicates the concentration is less than the report detection limit. -- = test not performed. L.T. = less than the amount specified. % = percent. ppm = parts per million. ppb = parts per billion. v/v = volume analyte/volume sample. w/w = weight analyte/weight sample.





ID: Air Products and Chemicals

21435-60-2

AAL Number: 13566-2

Volatile Sulfur Compound	ds (VSC, ppm v/v)	Result	<u>D.L.</u>
Hydrogen Sulfide (H <sub>2</sub> S):		7.1	0.1
Carbonyl Sulfide (COS):		nd	0.1
Sulfur Dioxide (SO <sub>2</sub> ):		nd	0.1
Methyl Mercaptan:		nd	0.1
Ethyl Mercaptan:		nd	0.1
Dimethyl Sulfide:		nd	0.1
Carbon Disulfide:		nd	0.1
Isopropyl Mercaptan		nd	0.1
t-Butyl Mercaptan:		nd	0.1
n-Propyl Mercaptan:		nd	0.1
Methyl Ethyl Sulfide:		nd	0.1
sec-Butyl Mercaptan:		nd	0.1
Thiophene:		nd	0.1
Isobutyl Mercaptan:		nd	0.1
Diethyl Sulfide:		nd	0.1
n-Butyl Mercaptan:		nd	0.1
Dimethyl Disulfide:		nd	0.1
3-Methylthiophene:		nd	0.1
Tetrahydrothiophene:		nd	0.1
2-Ethylthiophene:		nd	0.1
2,5-Dimethylthiophene:		nd	0.1
Diethyl Disulfide:		nd	0.1
Unknown Compounds:		nd	0.1

Comments: Total Sulfur = 7.1 ppm v/v (0.0007 % v/v).

**D.L.** = report detection limit.  $\mathbf{nd}$  = indicates the concentration is less than the report detection limit. -- = test not performed. **L.T.** = less than the amount specified. % = percent.  $\mathbf{ppm}$  = parts per million.  $\mathbf{ppb}$  = parts per billion.  $\mathbf{v/v}$  = volume analyte/volume sample.  $\mathbf{w/w}$  = weight analyte/weight sample. **Unit Conversions:** 1 ppm v/v = 1 $\mu$ L/L = 1,000 ppb = 0.0001% v/v.

Reviewed By,

Richard F. Frisch

Addendum: - Chromatograms on-file Notebook data on-file



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