Table 7-1 – Heat and Material Balance (continued)

Stream Description		Stripped Condensate Drum Overhead to Hydrogen Rich Fuel Gas Stream		Saturated LP Steam from HRSG LP Steam Drum to Condensate Stripper		CO2 Product from Sulferox Unit to CO2 Compressor Precooler		CO2 Product from CO2 Compressor Precooler to Compression Package		CO2 Product from Compressor 1st stage to Dryer Package	
Stream Number		66		67		68		69		70	
Temperature, °C		126		151		68		35		30	
Pressure, bara		2.4		4.8		30.6		30.3		49.6	
Component Flows	MW	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %
CH4	16.04	0	0.0%	0	0.0%	2	0.0%	2	0.0%	2	0.0%
H2O	18.02	67	99.1%	1,043	100.0%	70	1.1%	14	0.2%	8	0.1%
CO2	44.01	1	0.9%	0	0.0%	5,738	89.0%	5,738	89.7%	5,738	89.8%
H2	2.02	0	0.0%	0	0.0%	583	9.0%	583	9.1%	583	9.1%
N2	28.02	0	0.0%	0	0.0%	35	0.5%	35	0.5%	35	0.5%
CO	28.01	0	0.0%	0	0.0%	15	0.2%	15	0.2%	15	0.2%
H2S	34.08	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
COS	60.07	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
NH3	17.03	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
AR	39.95	0	0.0%	0	0.0%	8	0.1%	8	0.1%	8	0.1%
Total kgmol/hr		68	100.0%	1,043	100.0%	6,450	100.0%	6,394	100.0%	6,388	100.0%
Total kg/hr		1,233		18,793		256,683		255,674		255,568	
Molecular Weight		18.25		18.02		39.80		39.99		40.01	
Density, kg/m3		1.3		2.6		47.2		54.2		102.2	
Liquid Flow, m3/hr		-		-		-		-		-	
Vapor Flow, m3/hr		949		7,226		5,436		4,717		2,501	

Table 7-1 – Heat and Material Balance (continued)

Stream Description		CO2 Product from 1st Stage Intercooler to 2nd Stage of Compression		CO2 Product from 2nd Stage of Compression to Aftercooler		CO2 Product to Sequestration		Saturated LP Steam from HRSG LP Steam Drum to Sulferox SRU		Make-up Water to Sulferox SRU	
Stream Number		71		72		73		74		75	
Temperature, °C		30		77		30		151		60	
Pressure, bara		48.9		80.1		80.0		4.8		34.5	
Component Flows	MW	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %	kgmol/hr	mol %
CH4	16.04	2	0.0%	2	0.0%	2	0.0%	0	0.0%	0	0.0%
H2O	18.02	0	0.0%	0	0.0%	0	0.0%	220	100.0%	54	100.0%
CO2	44.01	5,738	89.9%	5,738	89.9%	5,738	89.9%	0	0.0%	0	0.0%
H2	2.02	583	9.1%	583	9.1%	583	9.1%	0	0.0%	0	0.0%
N2	28.02	35	0.5%	35	0.5%	35	0.5%	0	0.0%	0	0.0%
CO	28.01	15	0.2%	15	0.2%	15	0.2%	0	0.0%	0	0.0%
H2S	34.08	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
COS	60.07	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
NH3	17.03	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
AR	39.95	8	0.1%	8	0.1%	8	0.1%	0	0.0%	0	0.0%
Total kgmol/hr		6,380	100.0%	6,380	100.0%	6,380	100.0%	220	100.0%	54	100.0%
Total kg/hr		255,424		255,424		255,424		3,967		966	
Molecular Weight		40.04		40.04		40.04		18.02		18.02	
Density, kg/m3		100.3		139.1		213.2		2.6		959.1	
Liquid Flow, m3/hr		-		-		-		-		1	
Vapor Flow, m3/hr		2,547		1,836		1,198		1,526		-	

Table 7-1 – Heat and Material Balance (continued)

Stream Description		Sulfur Product		Condensate to Blowdown Sump				
Stream Number		76		77				
Temperature, °C		50		35				
Pressure, bara		1.0		30.3				
Component Flows	MW	kgmol/hr	mol %	kgmol/hr	mol %			
CH4	16.04	0	0.0%	0	0.0%			
H2O	18.02	21	53.8%	62	100.0%			
CO2	44.01	0	0.0%	0	0.0%			
H2	2.02	0	0.0%	0	0.0%			
N2	28.02	0	0.0%	0	0.0%			
CO	28.01	0	0.0%	0	0.0%			
H2S	34.08	0	0.0%	0	0.0%			
COS	60.07	0	0.0%	0	0.0%			
NH3	17.03	0	0.0%	0	0.0%			
AR	39.95	0	0.0%	0	0.0%			
Sulfur	32.06	18	46.2%					
Total kgmol/hr		39	100.0%	62	100.0%			
Total kg/hr		960		1,110				
Molecular Weight		24.62		18.02				
Density, kg/m3		-		984.3				
Liquid Flow, m3/hr		-		1				
Vapor Flow, m3/hr		-		-				

1.2.1.2 Production of Hydrogen Fuel by Sorbent Enhanced Water Gas Shift Reaction

Report Title

CO_2 Capture Project - An Integrated, Collaborative Technology Development Project for Next Generation CO_2 Separation, Capture and Geologic Sequestration

Production of Hydrogen Fuel by Sorbent Enhanced Water Gas Shift Reaction

Report Reference

1.2.1.2

Type of Report:	Semi-Annual Report
Reporting Period Start Date:	February 2003
Reporting Period End Date:	July 2003
Principal Author(s):	Jeffrey Hufton, Robert Chiang, Rodney Allam, Ed Weist, Vince White
Date Report was issued:	August 2003
DOE Award Number:	DE-FC26-01NT41145
Submitting Organization:	Air Products and Chemicals
Address:	7201 Hamilton Blvd Allentown, PA 18195

1.2.1.2.1 Abstract

This project is focused on the development of the Sorption Enhanced Water Gas Shift (SEWGS) process for decarbonizing syngas from an O_2 or air-based ATR to yield essentially CO_2-free H_2 fuel for power generation. The SEWGS process combines the water gas shift reaction with high temperature CO_2 removal via a solid adsorbent to simultaneously react CO to low levels and remove CO_2. A high pressure, high temperature H_2 product stream is produced which is used to generate power in a gas turbine, and waste heat is converted to power via steam turbines.

The overall goal of this work is to develop process flow sheets and equipment specifications for full power generation systems for both the Alaskan and Norcap scenarios of the CCP. This report primarily describes laboratory work carried out to define important characteristics of our best high temperature adsorbent (ADS2-1). Adsorption isotherms and adsorption/desorption characteristics have been evaluated. The adsorbent exhibits some unconventional behavior that makes description of the process with conventional adsorption simulators difficult. An alternative process design approach has therefore been formulated to generate SEWGS heat / mass balance estimates and equipment sizing. Future experiments will provide additional justification of the assumptions inherent in this approach. This design information will then be passed to an ASPEN process simulator for evaluation of the impact of the SEWGS on the power generation process.

1.2.1.2.2 Table of Contents

1.2.1.2.3 List(s) of Graphical Materials

1.2.1.2.4 Introduction

This report describes work on a new process concept combining the shift reaction and high temperature CO_2 adsorption to produce decarbonised hydrogen fuel for power production. The process is referred to as the shift-SER (shift Sorption Enhanced Reaction) process, or the SEWGS (Sorption Enhanced Water Gas Shift) process. Both acronyms have been used interchangeably in the past.

The development program has been supported through the Precombustion subgroup of the CCP (CO_2 Capture Program).

This report will describe laboratory efforts during the time period from February 03 through July 03. This time period is consistent with the end of Phase II of the program.

Simulation work carried out in Phase I of the program showed that implementation of the SEWGS process for fuel gas decarbonization could significantly reduce the cost of CO_2 removal compared to an amine-based process (Allam et al., 2002). Many potential high temperature adsorbents were considered in the beginning of Phase II (Allam et al, 2003). In this report, the adsorption/desorption characteristics of the most promising adsorbent materials (ADS1-2 and the adsorbent family ADS2; see paragraph 1, Appendix A for description) are investigated.

1.2.1.2.5 Executive Summary

Characterization of the adsorption/desorption properties of our best high temperature CO_2 adsorbent, ADS1-2, was the main task for this quarter. Performance was evaluated in the process test unit. Breakthrough curves were used to define the CO_2 adsorption isotherm at 400-500C. The isotherm was satisfactorily fit to a dual site Langmuir isotherm model. The temperature dependence of the CO_2 capacities was typical and characterized by a 10 kcal/mole heat of adsorption.

Mass transfer rates were inferred from the shape of adsorption and desorption profiles measured with the test unit at 400-500C. The adsorption mass transfer rate is fast, characterized by a mass transfer coefficient of at least 0.1 1/s. The desorption mass transfer coefficient is lower, but lack of consistency of the model with experimental data obtained at various purge gas flow rates makes it impossible to assign a mass transfer coefficient value.

The adsorption process model does not describe the impact of purge flow rate on the observed desorption data. Namely, experimental data indicate that desorption of CO_2 from ADS1-2 is rate limited. It also shows that the desorption process is not very sensitive to purge flow rate (the adsorption process model, however, is sensitive). Cyclic experiments also support this conclusion. The potential of using the adsorption process model to predict the SEWGS process performance is therefore low unless modifications are made to the underlying physics used in this model. These modifications are not planned for the future.

Unique sensitivity of cyclic performance was observed with process temperature. It was found that the cyclic CO_2 working capacities with the ADS1-2 adsorbent are not dependent on the process temperature. It appears that the decrease in CO_2 equilibrium capacity with temperature (observed via the isotherm data) is offset by an increase in CO_2 desorption rate.

An alternative approach has been taken to generate an approximate SEWGS process design from the experimental data. More experiments in the process test unit are needed to justify some of the assumptions in this procedure. The most important of these are associated with de-rating the CO_2 working capacity when a CO_2 rinse step is included in the process, sensitivity to purge gas velocity (or G-rate), impact of an axial temperature gradient along the SEWGS reactor, and evaluation of the required inventory of catalyst in the reactors. A series of experiments is planned to obtain input on these key topics. In addition, we are modifying our test unit to permit operation with syngas feed (containing H_2, CO), and will conduct reaction experiments to demonstrate the concept of SEWGS.

Incorporation of the SEWGS mass and energy balance data into the Alaskan and Norcap scenarios is underway (ASPEN modeling).

Catalyst activity testing of the ADS1-2 adsorbent was carried out to determine if catalyst could be omitted in the SEWGS beds. Preliminary results unfortunately indicate that there is no WGS catalytic activity at 400C or less. Catalyst will have to be included in the SEWGS beds along with the adsorbent.

Material development efforts have continued. An alternative adsorbent ASD2-1 was prepared that is more stable than previous versions. A scaled-up sample was produced and activated for testing in the process test unit. The desorption rate was found to be higher than in ADS1-2, but the lower equilibrium CO_2 capacity makes the cyclic working capacity, and hence the ASD2-1 adsorbent, inferior to the base ADS1-2 adsorbent.

1.2.1.2.6 Experimental

The experimental apparatuses used in this work include a modified high temperature TGA unit and a process test unit. Both have been thoroughly described in the recent report of Allam et al. (2003). Procedures for evaluating the results of these experiments are also available in that reference.

1.2.1.2.7 Results and Discussion

1.2.1.2.7.1 Material Development Work

More detailed information regarding materials work can be found in Section 1 of confidential Appendix A.

1.2.1.2.7.1.1 ADS1 Adsorbents

Efforts to improve the ADS1 and ADS2 adsorbents continued. An alternative formulation of ADS1, called ADS-3 was obtained from a vendor after a recent visit. This new material was bound with silica instead of the normal alumina-based binder (ADS1-1). The ADS-3 material was treated via our conventional procedure and tested in the TGA unit. The cyclic CO_2 capacity was slightly lower than the capacity of other ADS1 adsorbents. Thus, there appears to be no obvious advantage in capacity with the ADS1-3 adsorbent.

1.2.1.2.7.1.2 ADS2 Adsorbents

We prepared alternative formulations of ADS2-type adsorbents in the lab. The highest CO_2 capacity at 450C was 1.11% for material ADS2-1. The stability of ADS2-1 was investigated via an aging study by TGA. After ~300 cycles the stabilized capacity was 1.01%. We were very encouraged by the results and decided to scale-up the synthesis procedure to produce enough material for testing in the cyclic unit. A sample of the scaled-up batch had a CO_2 capacity of 1.17% by pristine activation in the TGA. The material was then activated in a pilot-scale air purged heater. The final activated ADS2-1 adsorbent exhibited an acceptable CO_2 capacity of 1.1%.

1.2.1.2.7.2 Adsorbent Testing in Fixed Bed Unit – ADS1-2 Adsorbent

The ADS1-2 adsorbent was evaluated in the process test unit to measure the adsorption isotherm, adsorption and desorption profiles, and cyclic performance.

As described by Allam et al. (2003), the adsorbent was subjected to multiple cycles of CO_2 adsorption and regeneration at 450C to age the material. The CO_2 adsorption capacity from these tests stabilized after 10-20 cycles. Isotherm and adsorption/desorption profile evaluations were then carried out.

A series of adsorption, depressurization, purge and pressurization steps were performed yielding effluent CO_2 mole fraction data illustrated in Figure 1. The feed time was long enough for CO_2 breakthrough, and regeneration was carried out to ensure that the CO_2 was desorbed before the next sequence. The adsorption capacity, used to define a point on the adsorption isotherm, was determined from the stoichiometric breakthrough time during the feed step. Void gas contributions were subtracted out via the results of void volume depressurization experiments described in Allam et al. (2003). The CO_2 mole fraction and flow rate data during the depressurization and purge steps were used to evaluate the amount of CO_2 removed during regeneration. These values were then normalized by the total amount of CO_2 initially in the column to yield the fraction of CO_2 removed (or f) and plotted versus the amount of purge gas introduced to the column. Overall and CO_2 mass balances were determined and typically found to be within 5%.

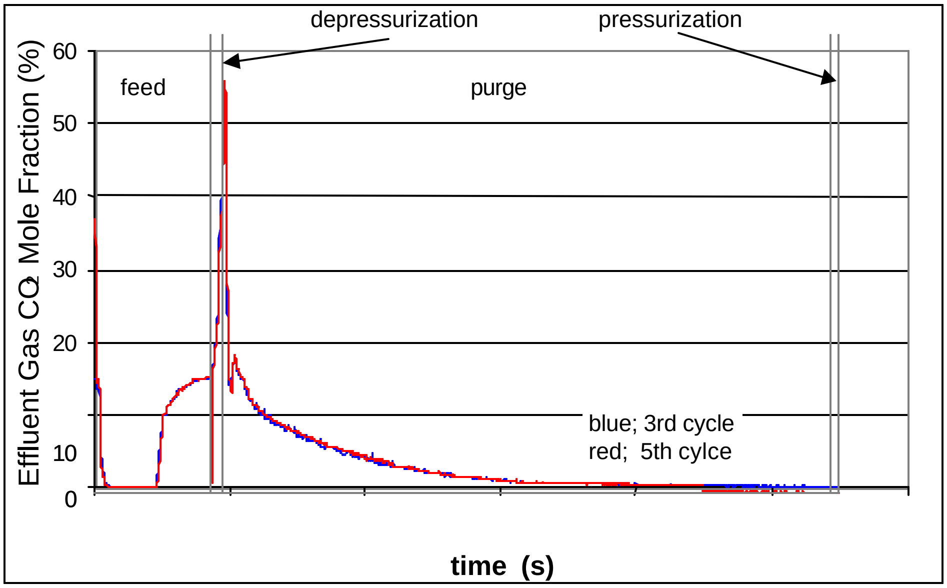


Figure 1. Effluent Gas CO_2 Mole Fraction During a CO_2 Feed, Depressurization, Purge, and Pressurization Cycle.

The CO_2 mole fraction data for repetitive experiments were found to be very reproducible, as evidenced by the results in Figure 1. This was true even after the adsorbent was removed from column, repacked, and run again.

1.2.1.2.7.2.1 CO_2 Adsorption Isotherm on ADS1-2

Additional data have been obtained since the last report (Allam et al., 2003) which help define the adsorption isotherm for CO_2 on ADS1-2 at temperatures of 400-500C. The isotherm is plotted in Figure 2. The 450C data were obtained with two different samples of the adsorbent, and very good agreement is observed. The trend with temperature is as expected for adsorption – higher temperature lowers the CO_2 adsorption capacity. The heat of adsorption (via the Clausius-Clapeyron equation) was found to be ~10 kcal/mole.

The fit of the nonisothermal dual-site Langmuir model to these data is also illustrated in Figure 2 (model results plotted as lines). The model captures the general trends of the data rather well. The model can be written as:

(1) $$n_{CO2} = \frac{m_1 b P_{CO2}}{1 + b P_{CO2}} + \frac{m_2 d P_{CO2}}{1 + d P_{CO2}}$$

where

(2) $$b = b_0 e^{q_1/RT}, d = d_0 e^{q_2/RT}$$

and n_{CO2} is in mmole/g and P is the partial pressure of CO_2 in atm. The parameter values are listed in Table A2 of Appendix A.

1.2.1.2.7.2.2 Measurement of Adsorption/Desorption Profiles

Adsorption and desorption profiles from runs similar to that presented in Figure 1 were investigated further. Breakthrough runs were carried out with feed gas containing 12.4% CO_2, 17.3% H_2O, and balance N_2 to simulate syngas from an air-based ATR. The column temperature was 450C and pressure

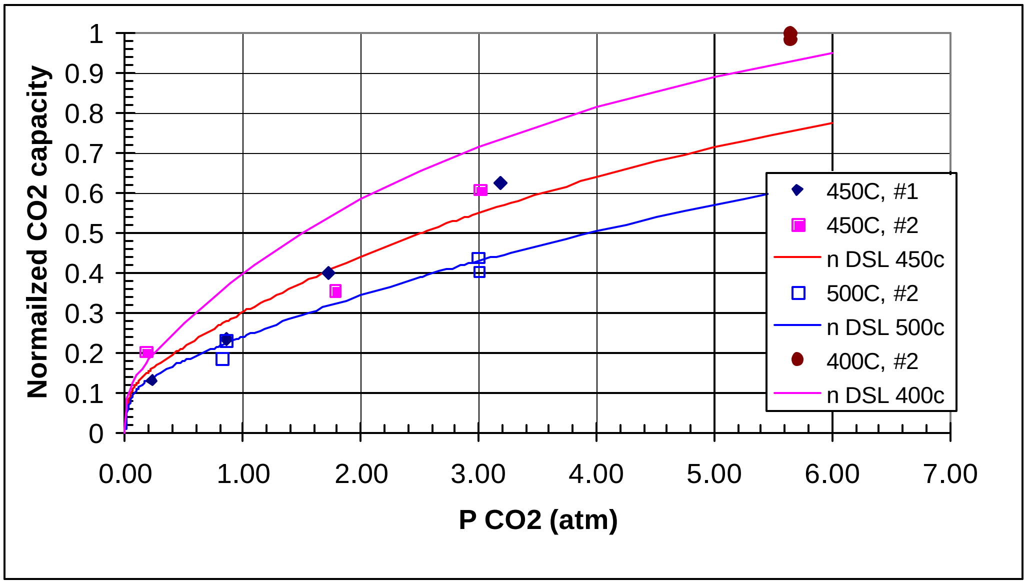


Figure 2. Adsorption Isotherm for CO_2 on ADS1-2; symbols – data, lines - model.

was 24.5 bar (355 psia). The feed gas rate was varied from 6.0 to 12.3 slpm (see paragraph 2 of Appendix A). The profiles are plotted in Figure 3 as the dry effluent CO_2 mole fraction versus normalized time (normalized so the curves intersect at t=0 when the effluent mole fraction is half the feed concentration). Reproducibility is excellent, as the data for multiple runs are essentially indistinguishable. The curve shapes are similar, with relatively rapid initial increases followed by slower approaches to the feed gas mole fraction (15.5% in this case). The slower increase is common when measuring breakthrough curves and can be due to heat effects or, in this case, perhaps due to two parallel adsorption processes with fast and slow kinetics. In either case, the time scale of our process requires characterization of the leading edge of the adsorption profile rather than the tail. Here the profile for the run made with higher feed rate is sharper than the lower flow rate. This is opposite expected behavior for a kinetically controlled adsorption process, since increased flow rate typically broadens the mass transfer zone. It was later determined that this effect is due to the dynamics of void volumes in the system (water knockout tanks) rather than adsorption kinetics. The adsorption kinetics are therefore too fast to directly measure at these conditions.

Carbon dioxide desorption curves are plotted in Figure 4. Effluent CO_2 mole fraction (dry) is plotted versus time for both the depressurization step and purge step. Before this test, the column was saturated with 12.4% CO_2, 17.3% H_2O, and balance N_2 at 450C and 24.5 bar (355 psia). The column was slowly depressurized (in countercurrent direction to feed gas flow) to ~1.7 bar (~25 psia), and then a constant purge flow was passed countercurrently for 2.5 hours. Purge flow rates of 3.4 and 6.9 slpm were used (see Paragraph 3 in Appendix A). The column pressure and temperature during this purge step were maintained at ~1.7 bar and 450C, respectively. As illustrated in the figure, the effluent CO_2 mole fraction increases rapidly during the depressurization step as CO_2 desorbs from the adsorbent, and then progressively decreases as the purge gas sweeps CO_2 from the column. Run to run reproducibility is again excellent. As expected, the profile for the slower purge rate is broader than for the higher purge rate.

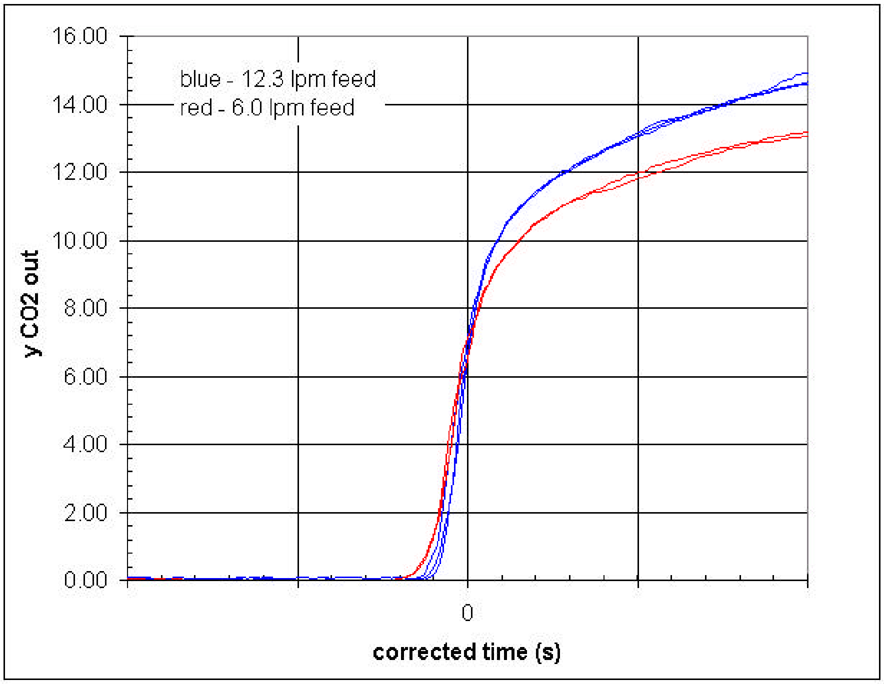


Figure 3. Adsorption Profiles for Breakthrough Runs with Different Feed Rate.

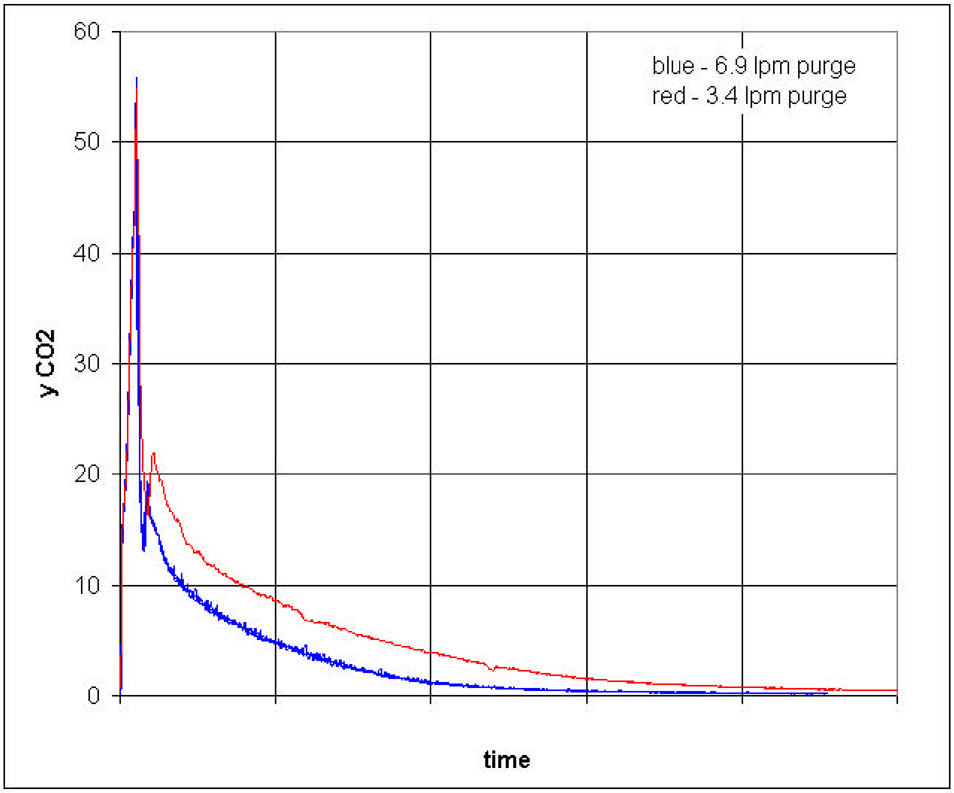


Figure 4. Desorption Data for CO_2 on ADS1-2 at 450C (Depressurization and Purge).

Regeneration of the adsorbent is one of the most critical steps in an adsorption process. Ideally, the rate of CO_2 desorption is fast and limited only by adsorption equilibrium limits. In this case, a minimum amount of purge gas is needed to remove CO_2 from the column. If the rate of CO_2 desorption is relatively slow, then more purge gas will be needed to remove a similar amount of CO_2. This yields higher costs for the process.

The efficiency of CO_2 removal can be characterized by determining the amount of purge gas needed to remove a given fraction of the CO_2 (both adsorbed phase and void gas). Figure 5 shows a plot of the fraction of CO_2 removed during regeneration (referred to as f) versus the normalized volume of purge gas fed to the column (see Figure A1 in Appendix A for alternative plot). The curves do not start from the origin since some of the CO_2 is removed via the depressurization step, which uses no purge gas. On this basis the data are rather similar, with only a slight inefficiency noted for the higher purge rate run (see Paragraph 4 of Appendix A).

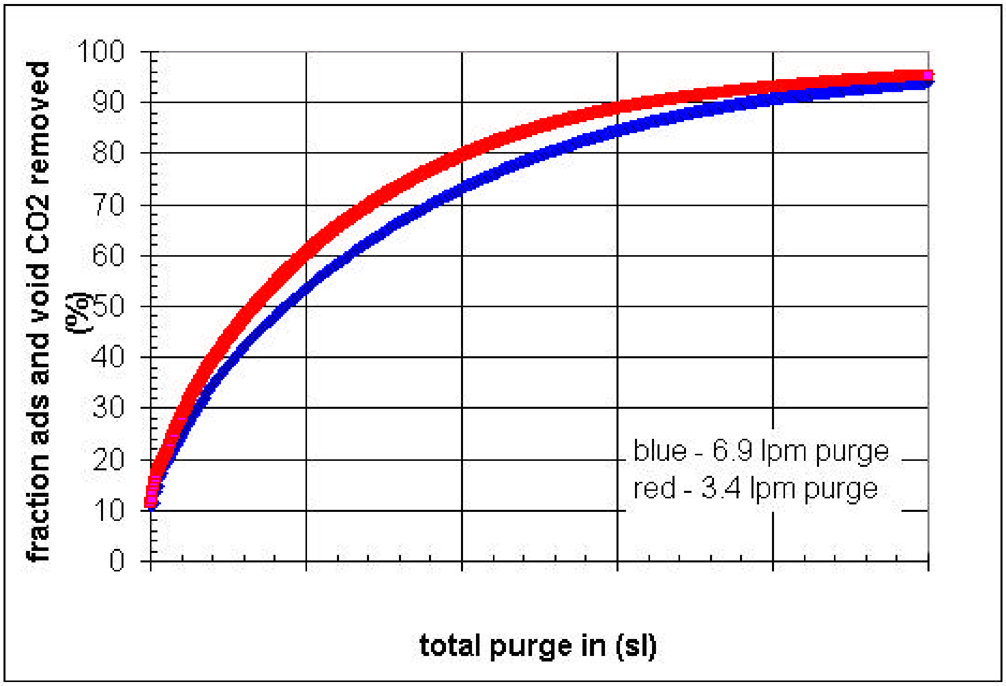


Figure 5. Plot of Fraction of CO_2 Removed During Regeneration.

1.2.1.2.7.2.3 Mass Transfer Rate Estimation

The adsorption and desorption profiles described above can in principle be fit with an adsorption dynamics model to determine mass transfer coefficients. The dual-site Langmuir isotherm was used to describe the system equilibrium, and a linear driving force model with constant mass transfer coefficients was used for mass transfer kinetics. Isothermal conditions were assumed in the model.

Accounting for experimental void volumes was found to be very important when modeling the adsorption breakthrough curves. Most of the dispersion was associated with mixing in these volumes rather than the adsorption mass transfer resistances. Hence, only a lower limit of the adsorption mass transfer coefficient could be estimated, which was found to be 0.1 1/s. A comparison of the model predictions with the experimental data are plotted in Figure 6 (see Figure A2 for alternative plot). The model with $k_{ads} = 0.1$ captures the shape of the leading edge of the profile for both feed flow rates - lower mass transfer coefficients yield broader mass transfer zones. (see paragraph 5 of Appendix A)

The adsorption dynamics model was next fit to the desorption data. The model must capture the dynamics of the depressurization process as well as CO_2 desorption during purge. Specification of the

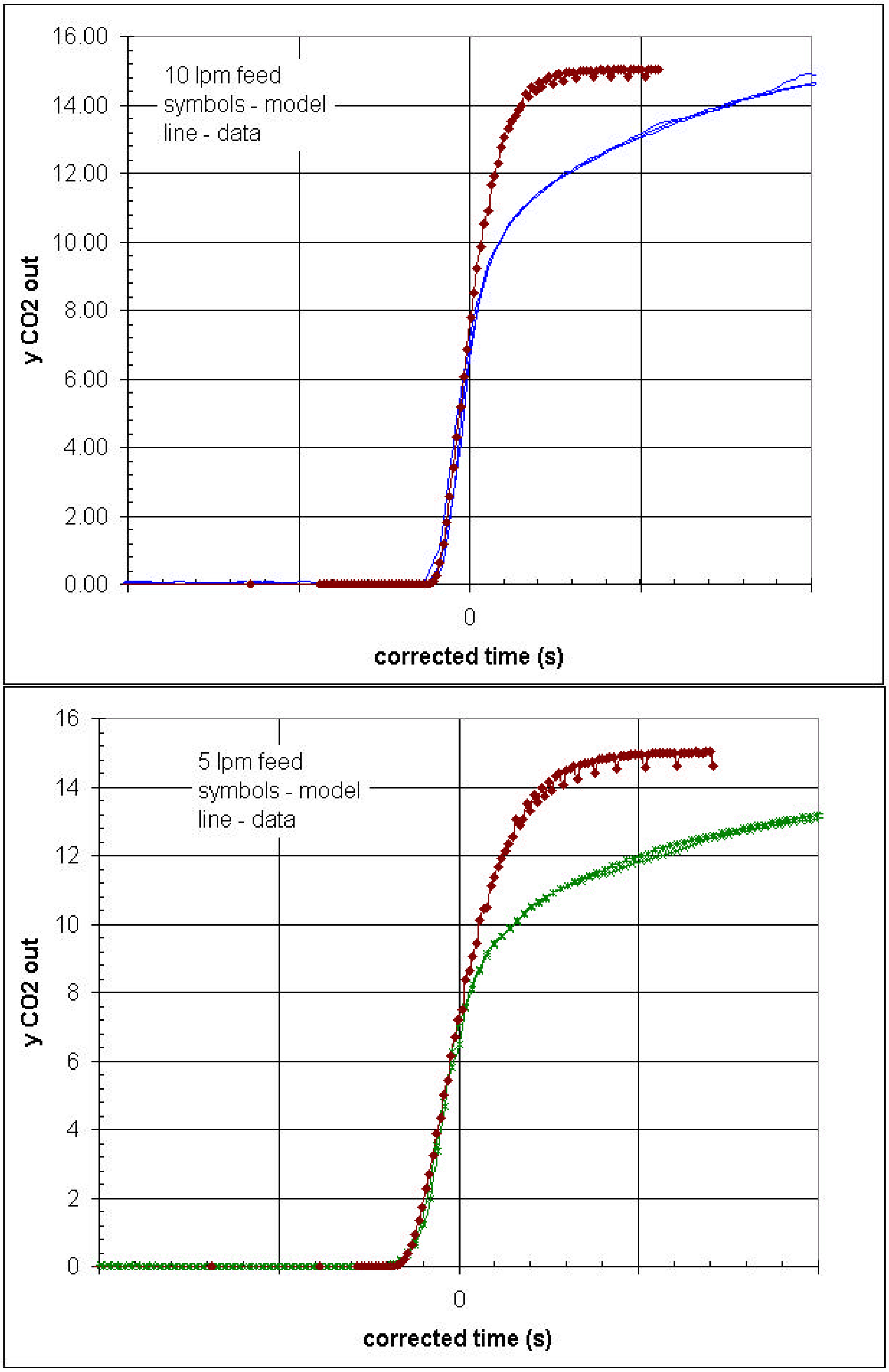


Figure 6. Comparison of Experimental Adsorption Profile with Model.

time-varying throttle valve Cv determines the depressurization effluent gas flow rate. Comparison of the model with the experimental flow data (6.9 lpm purge) are illustrated in Figure 7, and the agreement is very good.

The mass transfer coefficient for desorption, k_{des}, strongly effects the shape of the predicted desorption profile. A value of 0.1 1/s, found for the adsorption rate, was used to generate the model predictions illustrated in Figure 8. Clearly this mass transfer rate does not work. A best value for k_{des} was eventually determined (see paragraph 6, Appendix A). Comparison of the model prediction with the experimental data is plotted in Figure 9 (see Figure A4, Appendix A for alternative plot). The fit is reasonable, although this approach tends to weigh the long time portion of the curve, and does not necessarily describe the depressurization portion as well.

The model with the best value of k_{des} was used to predict desorption performance of the 3.4 lpm purge flow rate runs. The effluent flow rate data was well described, but the effluent CO_2 mole fraction data is less satisfying (Figure 10, and Figure A5, Appendix A). The model fails to capture the shape of the curve, particularly during the initial portion of the purge step.

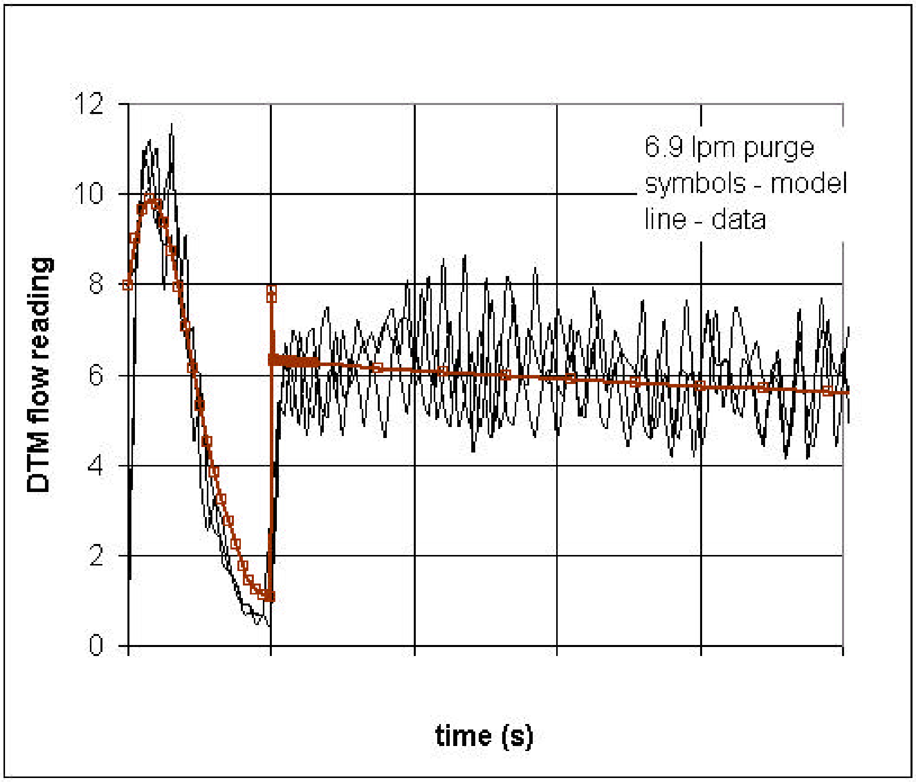


Figure 7. Comparison of Experimental Desorption Flow Rate with Model.

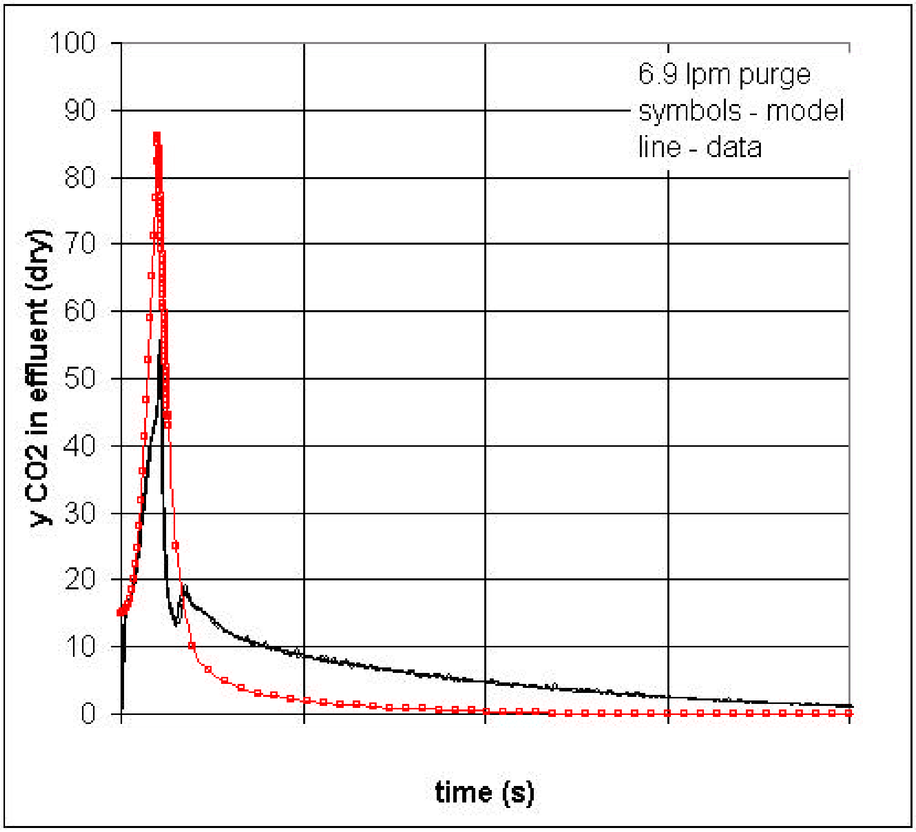


Figure 8. Comparison of Experimental Desorption Data with Model; k des = 0.1 1/s.

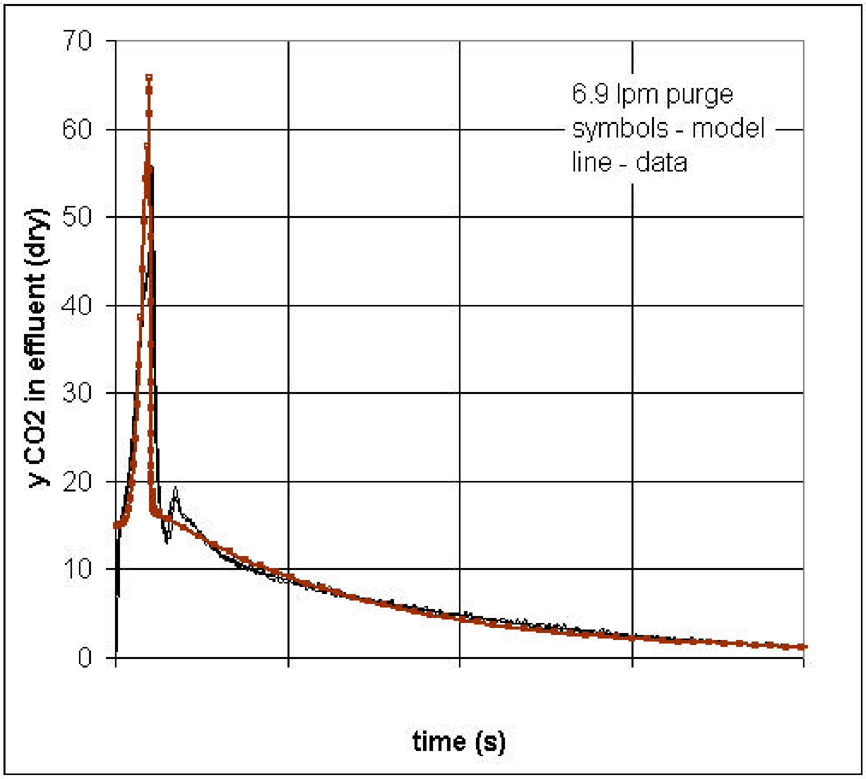


Figure 9. Comparison of Experimental Desorption Data with Model; best k des.

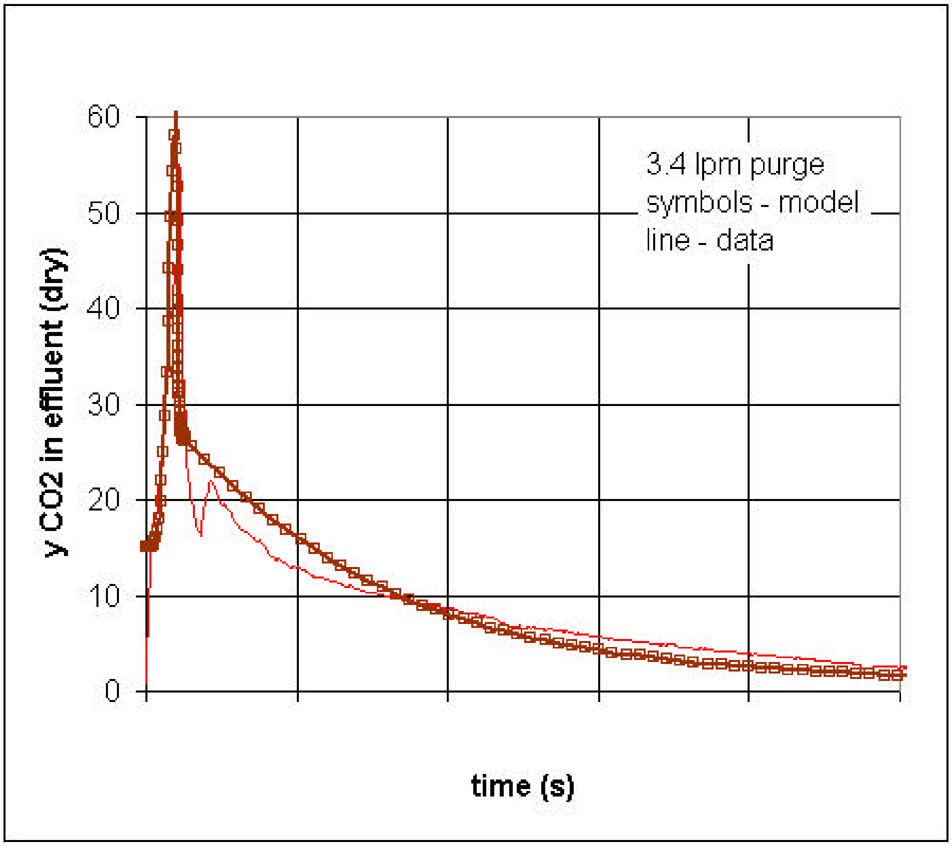


Figure 10. Comparison of Experimental Desorption Data with Model; best k des, 3.4 lpm purge.

An illustration of the experimental and model f-curves for both purge flow rates is presented in Figure 11. Clearly the f-curve for k_{des} = 0.1 1/s does not describe the data, as expected. This represents the ideal condition where mass transfer rates are high and desorption is limited by the adsorption isotherm (equilibrium). The f-curve generated with the best value of k_{des} describes the 6.9 lpm data relatively well, but fails to describe the 3.4 lpm data. The model predicts that doubling of the purge gas flow rate essentially doubles the amount of purge gas required for a given level of CO_2 removal. This is consistent with very slow mass transfer; the effect of purge flow on CO_2 desorption rate is minimal and the amount of CO_2 desorbed is essentially a function of time alone. Doubling the purge gas flow rate would then displace the f-curve of Figure 11 to the right by a factor of two, similar to the model predictions. The experimental data *do not* exhibit this same level of sensitivity to the purge gas flow rate. (see paragraph 7, Appendix A). Defining the source of this modeling discrepancy and modifying the model to account for it is perhaps possible, but difficult. This is one reason we decided to base our process design calculations on the best experimental data that we could obtain rather than use the adsorption process simulator (other reason described in Paragraph 8, Appendix A).

1.2.1.2.7.2.4 Cyclic Process Data

The process test unit was also operated in cyclic mode to evaluate the effective working capacity and adsorbed phase working capacity of the ADS1-2 adsorbent. The cycle consisted of a high pressure feed step with a mixture of CO_2, H_2O, and N_2; countercurrent (and throttled) depressurization to ~1.7 bar (25 psia); countercurrent purge; and countercurrent repressurization. The composition and flow rate of the effluent streams (product, depressurization, and purge) were continuously evaluated. Performance was determined by evaluating the N_2 product purity, the N_2 recovery (N_2 in product divided by N_2 in feed), and the CO_2 rejection (CO_2 in waste gas divided by CO_2 in feed). Working capacities included the effective CO_2 loading, calculated as the amount of CO_2 removed from the feed gas per mass of adsorbent in the vessel, and the adsorbed phase working capacity where the void gas contribution was subtracted out.

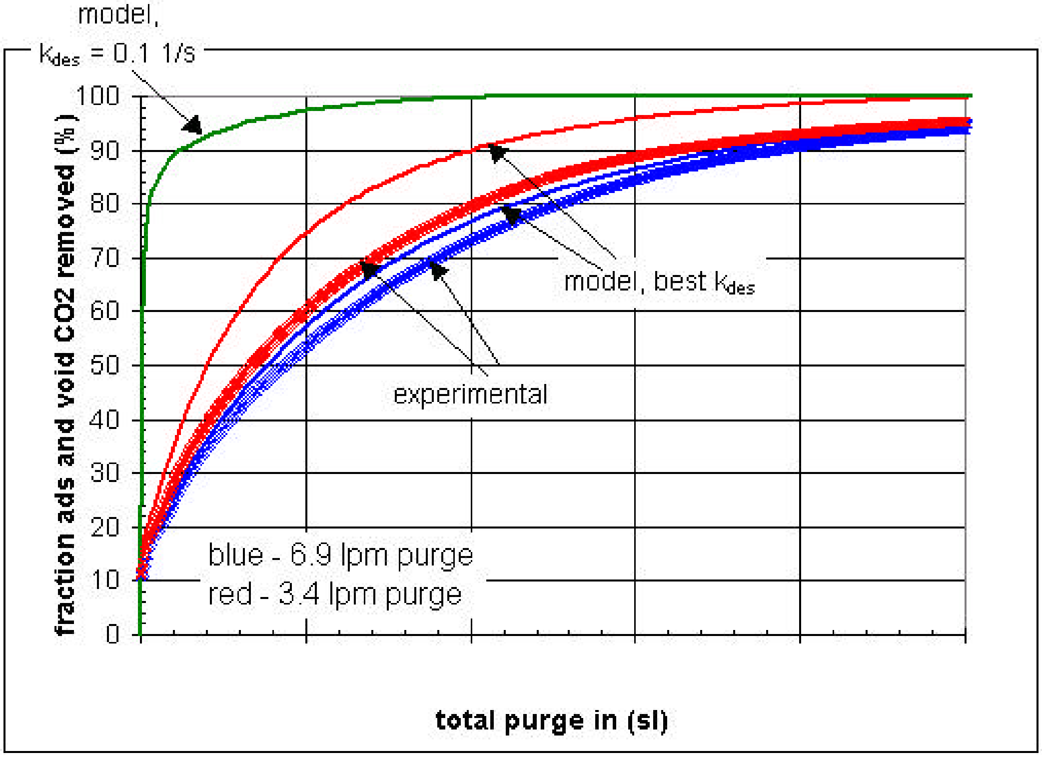


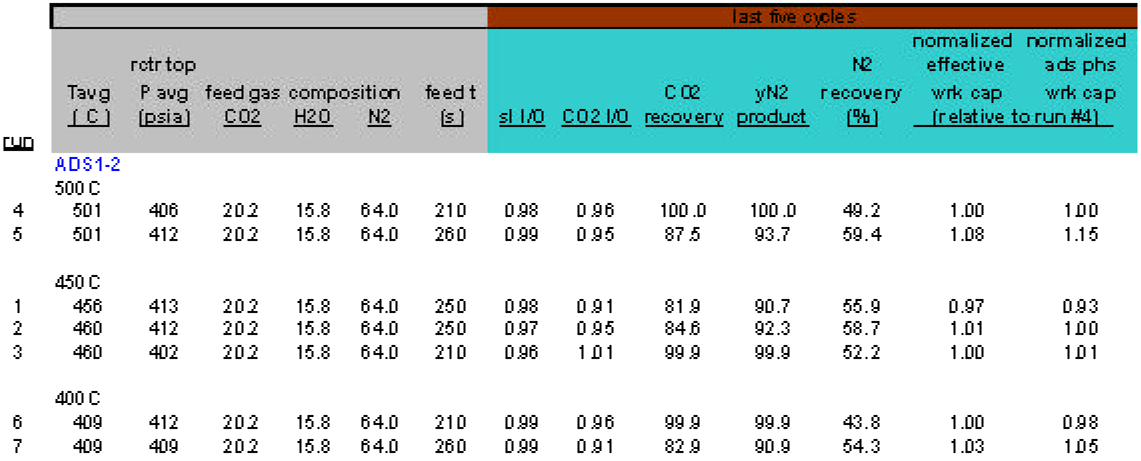
Figure 11. Comparison of Experimental and Model f Curves.

The results are listed in Table 3 (see Table A3 of Appendix A for more detail). All of the runs listed in this table utilized 20% CO_2 feed gas (simulates O_2-ATR syngas) at a feed pressure of ~28.3 bar (410 psia) and feed rate of 11.9 slpm. The cyclic runs were carried out in a manner that some CO_2 ended up in the product gas (3-10% CO_2). This ensures that the mass transfer zone is near the product-end of the column. Overall mass balances (see sl I/O) were all within 4%. Carbon dioxide balances (CO_2 I/O) were all within 10%, and more often than not were within 5%.

Runs 1-7 demonstrate the effect of process temperature on cyclic performance. For a fixed amount of purge gas (0.56 mmole purge/g adsorbent), the working capacity of the adsorbent remains constant for temperatures between 400 and 500C. The isotherm data clearly shows that the equilibrium CO_2 capacity decreases with increasing temperature. Thus, it appears that the mass transfer rate also increases with temperature in order to attain the same cyclic working capacities. From an adsorption point of view, there appears to be no advantage in operating the system at the higher temperatures.

Additional experiments were carried out to investigate the effect of purge time, purge gas velocity and composition, and depressurization time on cyclic performance. These data are described in Section 2 of Appendix A.

Table A3. Summary of Selected Cyclic Process Data.



							last five cycles						
run	Tavg (C)	rctr top P avg (psia)	feed gas composition CO2	H2O	N2	feed t (s)	sl I/O	CO2 I/O	CO2 recovery	yN2 product	N2 recovery (%)	normalized effective wrk cap (relative to run #4)	normalized ads phs wrk cap
	ADS1-2												
	500 C												
4	501	406	20.2	15.8	64.0	210	0.98	0.96	100.0	100.0	49.2	1.00	1.00
5	501	412	20.2	15.8	64.0	260	0.99	0.95	87.5	93.7	59.4	1.08	1.15
	450 C												
1	456	413	20.2	15.8	64.0	250	0.98	0.91	81.9	90.7	55.9	0.97	0.93
2	460	412	20.2	15.8	64.0	250	0.97	0.95	84.6	92.3	58.7	1.01	1.00
3	460	402	20.2	15.8	64.0	210	0.96	1.01	99.9	99.9	52.2	1.00	1.01
	400 C												
6	409	412	20.2	15.8	64.0	210	0.99	0.96	99.9	99.9	43.8	1.00	0.98
7	409	409	20.2	15.8	64.0	260	0.99	0.91	82.9	90.9	54.3	1.03	1.05

1.2.1.2.7.2.5 Process Evaluation

The first attempt at SEWGS process development based on the experimental results described above was to take the SEWGS model generated in Phase 1 (Allam et al., 2002) and modify it with the new isotherm model (Eqns. 1 and 2), an adsorption mass transfer coefficient of 0.1 1/s, and a desorption mass transfer coefficient obtained from the experiments. These calculations are relatively difficult (compared to conventional non-reactive PSA problems), oftentimes numerically crash, and generally take 2-4 days for convergence. Preliminary results indicate that the purge gas requirement increases by 20x over the base case from Phase I. Since the simulations do not completely describe the behavior of the experimental desorption data with varying purge rate, there is strong concern that this approach is not appropriate. We have therefore taken a more experimental approach in estimating process performance.

A first pass at estimating SEWGS performance from experimental data has been taken and is described in section 3 of Appendix A.

The process design is 'work in progress', and the following issues should be considered and addressed:

1. Impact of higher purge G-rate – use highest purge data available (which were unavailable at the time of model development), attempt to extrapolate CO_2 working capacity from lower G-rate data.
2. Impact of reactor temperature distribution – conduct desorption and cyclic runs with imposed temperature distribution from 350 to 500C along reactor to determine impact on working capacity and regeneration efficiency.
3. Impact of CO_2 rinse – carry out feed/rinse/depressurization/purge/repressurization experiments to evaluate impact of rinse on working capacity.
4. Impact of feed G-rate – thought to be relatively unimportant, but we could potentially increase the experimental feed flow rates to evaluate and perhaps extrapolate the effect.
5. Determine required inventory of catalyst via space velocity calculations with HTS activity equations, both with and without CO_2 removal.

In addition, we are committed to modification of our process test unit to enable operation with syngas feed. Demonstration of the SEWGS concept will then be carried out.

1.2.1.2.7.3 Adsorbent Testing in Fixed Bed Unit – ADS2-1 Adsorbent

The best formulation of ADS2 material (ADS2-1) was scaled up to allow testing in the process test unit. Repetitive breakthrough tests were carried out with 20.4% CO_2, 15.8% H_2O, balance N_2 at 400C and 28.3

bar (410 psia). The capacity fell during exposure and then stabilized at a value only 40% that of ADS1-2 (see paragraph 9, Appendix A).

The rate of desorption appears to be faster in the new adsorbent than in ADS1-2. Figure 12 illustrates desorption data for both (two runs with each material are plotted). The vertical line at an arbitrary purge volume intersects the ADS2-1 line at f= 44% compared to f=22% for ADS1-2. A constant portion of this CO_2 amount is due to void gas. With the void gas contribution eliminated, ADS2-1 removes 30% of the adsorbed CO_2, compared to 16% for ADS1-2.

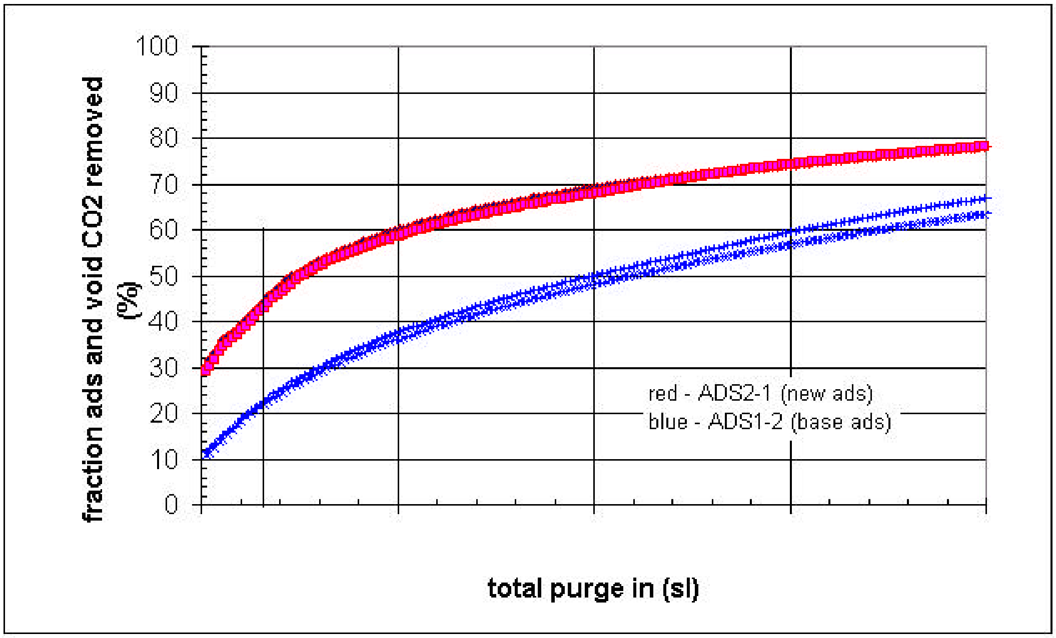


Figure 12. Fraction of CO_2 Removed during Regeneration by ADS2-1 and ADS1-2 Adsorbents.

Unfortunately, the low equilibrium CO_2 capacity of the ADS2-1 also impacts the total amount of CO_2 removed during the purge step. Figure 13 (Figure A8, Appendix A) illustrates the same data plotted as the normalized liters of CO_2 removed versus purge gas input. Here the higher final capacity of the ADS1-2 adsorbent is evident. The ADS2-1 adsorbent has a slight advantage at very low purge amounts, but then is outperformed by the base ADS1-2 adsorbent at higher purge volumes.

Cyclic data support these findings since the measured working capacities of the ADS2-1 are substantially inferior to those measured for ADS1-2. The current formulation of ADS2-1 does not hold promise for improved SEWGS performance (see paragraph 10, Appendix A).

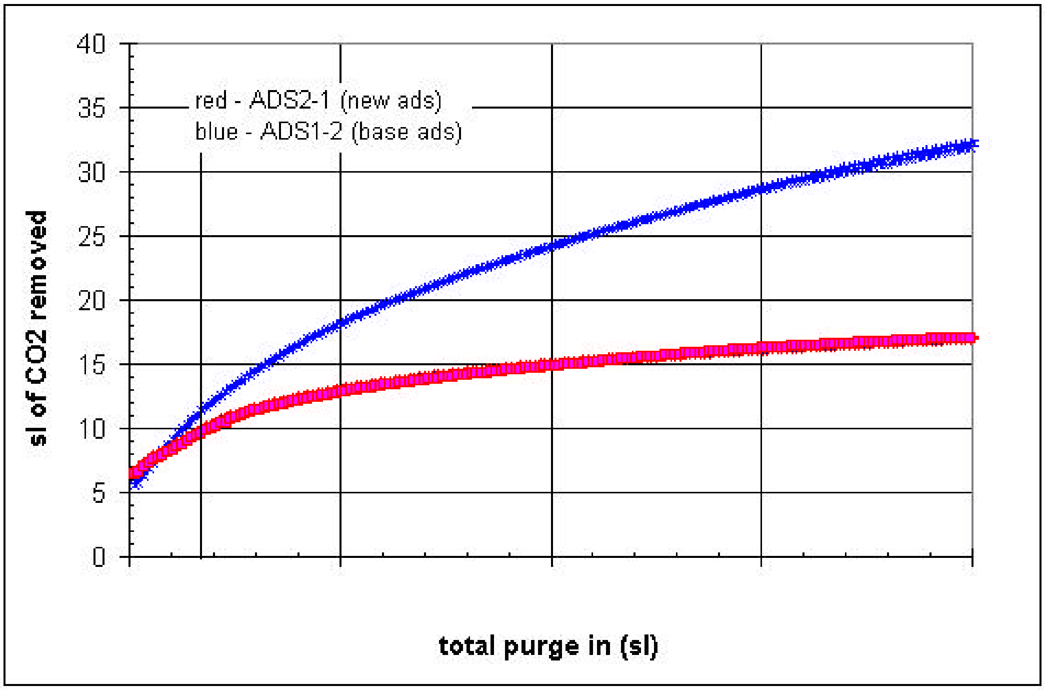


Figure 13. Standard Liters of CO_2 Removed during Regeneration by ADS2-1 and ADS1-2 Adsorbents.

1.2.1.2.7.4 High Temperature Valves for SEWGS

Jamesbury (now Metso Automation) valves were considered in the Phase I evaluation of the SEWGS process. Although discussions with sales personnel were promising (quotes were even provided), they have recently backed away from the application due to concern over the integrity of metal seals and bearings under the required combination of high temperature (550C, or 1020F) and frequent cycling (once every 5 minutes).

Four alternative vendors have been identified and solicited for quotes of feasibility and pricing for this application.

1.2.1.2.7.5 Catalytic Activity of ADS1-2 Adsorbent

Experiments have been carried out in our Catalysis group to determine if the ADS1-2 adsorbent has any intrinsic WGS catalytic activity. We have recently received a verbal report that it does not have activity at 400C. A full description will be disclosed in the next DOE report.

1.2.1.2.7.6 Alaskan and Norcap Scenario Process Evaluation

Work is underway to model SEWGS integrated with an ATR in order to provide hydrogen fuel for the two scenarios.

Norcap has been addressed in the past and is simply a matter of revising the work we did before but using the correct natural gas composition and using the latest SER parameters, which essentially boils down to the amount of steam required for regeneration.

The Alaska scenario is more complicated. In this case we are producing hydrogen to power some three different types of gas turbine. We have a model that predicts how much hydrogen fuel is required for these gas turbines. However, we are waiting for feedback from GE as to whether nitrogen injection will be required to satisfy NOx limitations.

We will be considering Air and Oxygen driven ATR. The hydrogen from the air ATR case contains nitrogen. The hydrogen from the oxygen ATR process does not contain nitrogen but this can be added since there will be nitrogen available from the ASU as required to meet NOx limitations.

1.2.1.2.8 Conclusion

The performance of the ADS1-2 adsorbent has been evaluated in the process test unit. The CO_2 adsorption isotherm has been determined and fit with a theoretical model. The temperature dependence of the CO_2 capacities is as expected and characterized by a 10 kcal/mole heat of adsorption. The adsorption mass transfer rate is fast, characterized by a mass transfer coefficient of at least 0.1 1/s. The desorption mass transfer coefficient is lower, but lack of consistency of the model with experimental data obtained at various gas flow rates makes it impossible to assign a mass transfer coefficient value.

Cyclic CO_2 working capacities with the ADS1-2 adsorbent are not dependent on the process temperature. It appears that the decrease in CO_2 equilibrium capacity with temperature is offset by a presumed increase in CO_2 desorption rate.

The ADS1-2 adsorbent does not have any intrinsic WGS catalytic activity. Catalyst will have to be included in the SEWGS beds along with the adsorbent.

The adsorption process model does not describe the impact of purge flow rate on the observed desorption data. Namely, experimental data indicate that desorption of CO_2 from ADS1-2 is rate limited, but the desorption process is not very sensitive to purge flow rate. Cyclic experiments also support this conclusion. The potential of using the adsorption process model to predict the SEWGS process performance is therefore low unless modifications are made to the underlying physics used in this model.

An alternative approach has been taken to generate an approximate SEWGS process design from the experimental data. More experiments in the process test unit are needed to obtain justification of some of the assumptions in this procedure. Incorporation of the SEWGS mass and energy balance data into the Alaskan and Norcap scenarios is underway.

An alternative high temperature CO_2 adsorbent (ADS2-1) has been prepared that is more stable than previous versions of this material. The desorption rate from this adsorbent is higher than ADS1-2, but the lower equilibrium CO_2 capacity makes the cyclic working capacity, and hence the ADS2-1 adsorbent, inferior to the base ADS1-2 adsorbent.

Additional conclusions are listed in Paragraph 12 of the Limited Rights Data Appendix.

1.2.1.2.9 References

Allam, R.J., Chiang, R.L, Hufton, J.R., Weist, E.L., and White, V., “Sorption Enhanced Shift Reaction with CO_2 Removal Project Phase II(a) Report, March 02- January 03, confidential semiannual report submitted to DOE (2003).

Allam, R.J., Chiang, R.L, Hufton, J.R., Tsao, T.-C.R., Weist, E.L., and White, V., “Sorption Enhanced Shift Reaction with CO_2 Removal Project Phase I Report, confidential Phase I report submitted to DOE (2002).

1.2.1.2.10 List of Acronyms and Abbreviations

TGA	Thermal Gravimetric Adsorption
SEWGS	Sorption Enhanced Water Gas Shift process (also called shift-SER)
HTS	high temperature shift
WGS	water gas shift

1.2.1.3 Compact Reformer with Advanced Pressure Swing Adsorption System for Hydrogen Fuel Production

Report Title

CO_2 Capture Project - An Integrated, Collaborative Technology Development Project for Next Generation CO_2 Separation, Capture and Geologic Sequestration

Compact Reformer with Advanced Pressure Swing Adsorption System for Hydrogen Fuel Production

Report Reference

1.2.1.3

Type of Report:	Semi-Annual Report
Reporting Period Start Date:	February 2003
Reporting Period End Date:	July 2003
Principal Author(s):	Paul Hurst
Date Report was issued:	August 2003
DOE Award Number:	DE-FC26-01NT41145
Submitting Organization:	BP Exploration
Address:	Building H, Chertsey Road Sunbury-on-Thames, TW16 7LN United Kingdom

1.2.1.3.1 Abstract

The CCP will develop new and novel technologies to reduce the cost of capturing CO_2 from large industrial combustion sources. Targets have been established for a 50% reduction in the cost to capture CO_2 from existing (retrofit) facilities and a 75% reduction from new-build facilities. To measure progress towards these goals, cost estimates for the application of the technologies must be developed which are prepared on a common, consistent, and comparable basis.

The CCP has defined a number of ‘scenarios’ (combinations of fuel burning equipment and fuel types) that are commonly found in its operations. The scenarios include:

1. Large gas-fired turbine combined-cycle power plant;
2. Distributed small/medium simple cycle gas turbines;
3. Refinery heaters and boilers;
4. Petroleum coke gasification.

The main objective of the technology developers will be to prepare process engineering designs and associated cost estimates that allow the technology under development to be compared with other technologies under consideration, on a transparent and comparable basis. The designs and associated costs developed will also be bench marked against a series of baseline studies, developed by the CCP using conventional CO_2 capture technology.

The focus of this study will be the Pre-Combustion capture of CO_2 via the Hydrogen production route.

The study will incorporate two distinctive technologies:

- Compact Reforming – Davy Process Technology
- Gemini Pressure Swing Adsorption (PSA) – Air Products Limited

The aim of the study is to develop a process design and associated cost estimate that integrates the Reforming and Adsorption units into a single process for the production of Hydrogen with the co-incident capture of CO_2 within scenario 3 (Refinery heaters and boilers).

The study aim is to capture 2.0 million tonnes per annum of CO_2 by utilizing refinery fuel gas streams as feed to the combined Reformer/PSA unit and subsequently utilizing the produced Hydrogen as a substitute fuel in the refinery heaters and boilers. The CO_2, captured as a pressurized product from the Gemini PSA unit, will be further compressed for export for use in an offshore enhanced oil recovery scheme.

1.2.1.3.2 Table of Contents

1.2.1.3.3 Experimental

This study is entirely a paper exercise; there will be no work of an experimental nature undertaken.

Key outputs will be an engineering design study report and associated cost estimate based upon a plant design optimised for the Refinery heaters and boilers scenario.

Davy Process Technology will design and engineer the Compact Reformer section based upon their licensed design. This will be integrated with an Air Products Gemini PSA unit to optimise the overall energy performance and thermal efficiency of the system.

Both companies will provide engineering cost estimates for their respective sections based upon the agreed/optimised design.

1.2.1.3.4 Results and Discussion

This study is still in the contract negotiation phase and there are no results to report.

1.2.1.3.5 Conclusion

This study is still in the contract negotiation phase and there are no conclusions to report.

1.2.1.3.6 References

This study is still in the contract negotiation phase and there are no references to quote.

1.2.2. Coke Gasification

1.2.2.1 Advanced Technology For Separation and Capture of CO_2 From Gasifier Process Producing Electrical Power, Steam and Hydrogen

Report Title

CO_2 Capture Project - An Integrated, Collaborative Technology Development Project for Next Generation CO_2 Separation, Capture and Geologic Sequestration

Advanced Technology for Separation and Capture of CO_2 from Gasifier Process Producing Electrical Power, Steam and Hydrogen

Report Reference

1.2.2.1

Type of Report:	Semi-Annual Report
Reporting Period Start Date:	February 2003
Reporting Period End Date:	July 2003
Principal Author(s):	Valerie Francuz and Satish Reddy
Date Report was issued:	August 2003
DOE Award Number:	DE-FC26-01NT41145
Submitting Organization:	Fluor Federal Services Inc.
Address:	One Fluor Daniel Drive Aliso Viejo, CA 92698 USA

Fluor Disclaimer

"This non-confidential report was prepared for the CO_2 Capture Project (CCP) by Fluor Enterprises Inc. and other consultants (i.e. equipment vendors) and is based in part on information not within the control of either the CCP, Fluor or the consultants. Neither Fluor nor the consultants have made an analysis, verified, or rendered an independent judgment of the validity of the information provided by others. While it is believed that the information contained herein will be reliable under the conditions and subject to the limitations set forth herein, neither Fluor nor the consultants guarantee the accuracy thereof. Use of this report or any information contained therein shall constitute a release and agreement to defend and indemnify Fluor and such consultants from and against any liability (including but not limited to liability for special, indirect or consequential damages) in connection with such use. Such release from and indemnification against liability shall apply in contract, tort (including negligence of Fluor or such consultants, whether active, passive, joint or concurrent), strict liability, or other theory of legal liability; provided, however, such release, limitation and indemnity provisions shall be effective to, and only to, the maximum extent, scope or amount allowable by law.

Notwithstanding the above, neither this report nor any information contained therein or otherwise supplied by Fluor in connection with the Study and the Services shall be released by CCP other than that as permitted by the Study contract or used in connection with any proxy, proxy statement, proxy soliciting material, prospectus, Securities Registration Statement or similar document without the express written consent of Fluor, except as may be required by law. Further, CCP shall not use the name of Fluor without its prior written consents.

The information presented in this report contains data relating to the Texaco Gasification Process, Fluor CO_2LDSep^{SM} Technology and Fluor proprietary Sulfur Recovery Technology. The report has been prepared by FLUOR for the CCP consortium, which comprises the following member companies: British Petroleum, ChevronTexaco, ENI, Norsk Hydro, EnCana, Shell, Statoil and Suncor Energy. This report and the data contained therein may be shared amongst members of the CCP consortium."

1.2.2.1.1 Abstract

Phase I for this project developed a conceptual process and engineering design case for an advanced technology case for the Canadian Petroleum Coke Scenario Baseline Study in sufficient detail to determine a capital cost estimate with a ±40% accuracy. This work was commissioned by the Pre-Combustion team of the CO_2 Capture Project (CCP), a consortium of eight energy companies (British Petroleum, ChevronTexaco, ENI, Norsk Hydro, EnCana, Shell, Statoil, and Suncor Energy).

This advanced case is based on Fluor's CO_2LDSep^{SM} technology and consists of a conventional Integrated Gasification Combined Cycle (IGCC) plant with export steam, hydrogen, and electrical power. The plant also includes process steps to remove most of the carbon-containing components in the fuel gas prior to combustion in the gas turbine.

The total carbon capture of this plant is 88% (versus 90% for the baseline case) with an increased electrical power production of approximately 40 MWe over the Controlled Baseline Case. The total installed cost for the plant will be provided later.

1.2.2.1.2 Table of Contents

1.2.2.1.3 List(s) of Graphical Materials

1.2.2.1.4 Introduction

1.2.2.1.4.1 Project Background

Eight energy companies (British Petroleum, ChevronTexaco, ENI, Norsk Hydro, EnCana, Shell, Statoil, and Suncor Energy) have joined together to form the CO_2 Capture Project (CCP). The goals of the CCP include the development of new and novel technologies to decrease the amount of carbon dioxide emissions from large industrial sources. The goals of the advanced technologies are:

- to capture at least 90% of the carbon dioxide that would be emitted by a given facility; and
- to reduce the cost of carbon dioxide capture and storage by 75% for new facilities and 50% for retrofits when compared to the cost of achieving the same level of removal using currently available technologies.

The CCP seeks to develop technologies to the 'proof of concept' stage by the end of 2003. Thereafter, demonstration tests can be conducted to verify performance and cost estimates, and a large-scale application could be in operation before 2010.

In addition to the CCP member companies, financial support is also provided by the United States (U.S.) Department of Energy, the European Union, and Norwegian Klimatek Agencies for the reduction of carbon dioxide emissions.

The CCP has identified four scenarios, which represent existing or future planned facilities. The scenarios include: large gas-fired combined-cycle power plants, a distributed array of small/medium simple cycle combustion turbines, petroleum coke gasification plants, and refinery heaters and boilers (feed includes a variety of mixed liquid and gaseous fuels). On the carbon dioxide side, the CCP is divided into the following specialized technical teams:

- Post-Combustion – Carbon dioxide is removed from the exhaust gas from furnaces, boilers, combustion turbines, etc. This technology is commercially proven and can be retrofitted to existing equipment.
- Pre-Combustion – Carbon is removed from the fuel gas before combustion in the furnaces, boilers and combustion turbines.
- Oxyfuels – Oxygen is separated from the air and is used to combust hydrocarbons to produce an exhaust containing carbon dioxide and water (no nitrogen). The water can be easily condensed, leaving a highly concentrated carbon dioxide stream for storage.

Baseline studies shall be developed for each scenario to provide input to an economic model. This economic model will be used to prioritize and measure the extent of cost savings for future technology development options. Each baseline study will consist of a process design based upon the distinct scenario and individual site-specific requirements. The designs will use state of the art gas processing technology to reflect current best practice.

This study (an advanced technology case for the Canadian Petroleum Coke Scenario Baseline Study) has been initiated by the Pre-Combustion team, which has a specific focus on the capture and separation of carbon dioxide from fuel before combustion.

1.2.2.1.4.2 Scope of Work

The scope of this study (Phase I) is to create one advanced conceptual process and engineering design in sufficient detail for the development of a capital cost estimate with a ±40% accuracy. Several advanced technologies (membrane water gas shift reactor, Gemini PSA, etc.) were considered by CCP for study and were discarded from this effort (see separate CCP write-up for details). Therefore, for this project, the Advanced Case is based on Fluor's CO_2LDSep^{SM} technology and is analogous to the Controlled Baseline Case discussed in the Canadian Petroleum Coke Scenario Baseline Study. This advanced case consists of a conventional Integrated Gasification Combined Cycle (IGCC) plant with export steam, hydrogen, and electrical power, and also includes advanced processing steps to remove most of the carbon-containing components in the fuel gas prior to combustion in the gas turbine. The Advanced Case is designed for a total carbon capture of 88% (the Controlled Baseline Case has a carbon capture of 90%). The performance and cost basis for the Gasification Island were provided by ChevronTexaco.

The purpose of evaluating this Advanced Case is to:

1) learn how best to integrate this new technology into a conventional IGCC scheme
2) determine the reduction of carbon dioxide capture cost that can be obtained by using this advanced technology and
3) elucidate process performance and cost goals the advanced technology must meet in order to deliver on the CCP cost reduction targets (75% for new facilities and 50% for retrofits)

Following is a summary of the major activities for this study for the Advanced CO_2LDSep^{SM} Case:

1.2.2.1.4.2.1 Process

Fluor developed a process design, which incorporates the following key objectives:

- Cost effectiveness of the design.
- Flexibility of the design for turndown.
- Support systems (offsites and utilities) for a standalone project.

The results of the process design effort are presented in the following deliverables:

- Summary block flow diagram
- Preliminary process flow diagrams
- Heat and material balances
- Preliminary equipment lists with approximate sizes
- Cost estimate with a ±40% accuracy

Further evaluation of the advanced case will be provided later in Phase II of this study.

1.2.2.1.4.2.2 Cost Estimate

The capital cost estimate with at least a ±40% accuracy was prepared using an Icarus 2000 computer program. Pricing for special equipment was manually input based on Fluor equipment pricing database or budgetary quotations from vendors.

1.2.2.1.4.3 Scope of Facilities

The IGCC plant consists of the following units:

- Air Separation Unit
- Gasification Island
- Low Temperature Gas Cooling Unit
- Condensate (Ammonia) Stripper Unit
- CO_2LDSep^{SM} Unit
- Sulfur Recovery (Claus) and Tailgas Treating Unit
- Shift Reactors Unit
- Fuel Gas Saturator Unit
- Combustion Turbine and Heat Recovery Steam Generator Unit
- Steam Turbine and Condensate System
- Utilities & supporting systems include:

    - Natural gas supply
    - Demineralized water package
    - Cooling water package
    - Potable water package
    - Oily water separator
    - Fire protection and monitoring systems
    - Back-up plant and instrument air package
    - Wastewater treatment package (includes drains and sewer)
    - Flare system
    - Miscellaneous material handling system
    - Electrical distribution
    - Uninterruptible power supply (UPS)
    - Generator step-up transformer
    - Continuous emissions monitoring system (CEMS)
    - Distributed control system (DCS)
    - Interconnecting piping
    - Other supporting facilities (Process analyzers; Hazardous gas detection system; Communications; Control room; Maintenance, warehouse and administration facility; Laboratory for inspection, certification and process control; Turbine building; Overhead turbine crane; Heating, ventilation and air conditioning (HVAC) systems; and Roads, parking, fencing and lighting)

1.2.2.1.5 Executive Summary

1.2.2.1.5.1 Facility Summary Description

The Advanced CO_2LDSep^{SM} Case is based on feeding petroleum coke produced by the bitumen production and upgrading facility at Suncor's Oil Sands operations in Northern Alberta, Canada. The Integrated Gasification Combined Cycle (IGCC) plant produces hydrogen for use in hydroprocessing, steam for in-situ bitumen extraction using steam-assisted gravity drainage (SAGD) technology, electrical power, and carbon dioxide for onshore enhanced oil recovery (EOR) in Central Alberta. The capacity (petroleum coke feed flow rate) of the plant was set to be the same as the Controlled Baseline Case.

1.2.2.1.5.2 Key Results

The key results (performance and cost summaries) for the Advanced and Controlled Baseline Cases are shown in Table 1.2.2.1.5.2(1).

Table 1.2.2.1.5.2 (1) Performance and Cost Summary

	Controlled Baseline Case	**Advanced Case (CO_2LDSep^{SM})**
Basis		
Feed	Petroleum Coke	
Number of Combustion Turbines (General Electric 7FA)	3	
Site Conditions		
Dry Bulb Temperature, °C	2.8	
Barometric Pressure, mbara	950	
Relative Humidity	68%	
Performance		
Petroleum Coke Feed Rate, mt/d	6863	
Total Oxygen Feed Rate, mt/d (100% O2)	7289	7105
Sulfur Product, mt/d	387	
Power Summary, MWe		
Combustion Turbines	588	
Steam Turbine	181	176
Fuel Gas Expander	6	10
Auxiliary Power Consumption	340	300
Net Plant Output	435	474
Export Streams		
Hydrogen, Nm3/hr (MMSCFD)	67,000 (60)	
Steam, kg/hr (MMlb/hr)	589,600 (1.3)	
Carbon Dioxide, million mt/yr (100% capacity)	6.8	6.44
Carbon Dioxide Capture (@ 100% capacity)		

Table 1.2.2.1.5.2 (1) Performance and Cost Summary

	Controlled Baseline Case	**Advanced Case (CO_2LDSep^{SM})**
Carbon Dioxide Emitted, million mt/yr	0.6	0.85
Carbon Dioxide Recovered, million mt/yr	6.8	6.44
Carbon Recovery	91%	88%
Cost Estimate (2003 US Dollars)		
Accuracy	-15% to +30%	±40%
Total Installed Cost, $MM	1,364	To be provided later

1.2.2.1.6 Experimental

No experimental methods were required for this study. Instead, computer simulation was performed to determine the performance of the Integrated Gasification Combined Cycle based on a CO_2LDSep^{SM} Unit for carbon capture.

1.2.2.1.7 General Design Criteria

1.2.2.1.7.1 Introduction

This section presents the General Design Criteria for the Canadian Petroleum Coke Scenario, Advanced Case for CO_2 Capture Project. The scope of this conceptual study is to develop a process design and capital cost estimate with a ±40% accuracy for the gasification of petroleum coke to produce hydrogen, steam, electrical power and carbon dioxide based on Fluor's proprietary CO_2LDSep^{SM} technology.

The purpose of this section is to ensure a degree of uniformity of criteria for the design of the plant.

1.2.2.1.7.1.1 Brief Project Facilities Description

The following is a brief description of the Advanced CO_2LDSep^{SM} Case. Petroleum coke is slurried with water and gasified with oxidant (99.5 mol% oxygen) from the Air Separation Unit (ASU) to produce a raw syngas. The syngas from the gasifier is cleaned of particulates, preheated, shifted and cooled to a temperature suitable for the CO_2LDSep^{SM} Unit. Sulfur compounds are removed in the CO_2LDSep^{SM} unit and recovered as elemental sulfur product in the Sulfur Recovery unit. The carbon dioxide is recovered and a hydrogen rich stream is produced for fuel gas to the combustion turbines and hydrogen export. The carbon dioxide is compressed and dehydrated for Enhanced Oil Recovery (EOR).

The feed rate of petroleum coke is determined by recovering 67,000 Nm^3/hr (60 MMSCFD) of hydrogen from the IGCC and fully loading three General Electric Frame 7241(FA) combustion turbines (same feed flow rate as the Controlled Baseline Case). The hydrogen rich fuel gas mixture is diluted with nitrogen from the ASU to control NOx formation in the combustion turbine. Heat is recovered from the combustion turbine flue gas to produce steam. The steam is fed to a steam turbine to produce additional electrical power. The parasitical power consumers of the IGCC plant are satisfied from the gross electrical power produced with the remaining electricity sent for export.

The performance and cost basis for the Gasification Island were provided by ChevronTexaco.

1.2.2.1.7.1.2 General Criteria and Philosophy

a) The plant is designed to produce 67,000 Nm^3/h (60 MMSCFD) of hydrogen, 589,600 kg/hr (1.3 million lb/hr) of steam, and electrical power.

b) The plant is designed to capture 88% of the carbon in the feedstock as product carbon dioxide for enhanced oil recovery (EOR).

c) The steam export (589,600 kg/hr) is used for steam-assisted gravity drainage (SAGD) technology for the in-situ recovery of bitumen and losses must be made up by fresh make-up water.

d) The plant is designed to be self sufficient in all utilities including electrical power.

e) The plant is designed to have an operational life of at least 25 years.

1.2.2.1.7.1.3 Battery Limits Definition

The following commodities are supplied to the IGCC plant at the battery limits:

- Petroleum coke feed from petroleum coke stockpile
- Make up water
- Ambient air
- Water treatment chemicals
- Chemicals for the gasification unit

The following commodities are produced from the IGCC plant at the battery limits:

- Dry carbon dioxide product
- Hydrogen export
- Steam export
- Electrical power export
- Sulfur product
- Treated wastewater suitable for disposal
- Slag suitable for disposal/sale
- Fine slag suitable for disposal
- Sulfur recovery vent gas
- Air Separation Unit vent gas
- Flue gas
- Cooling tower evaporation
- Cooling tower drift (water droplets carried by the wind)
- Sewage
- Storm Drains

1.2.2.1.7.2 Site Data

1.2.2.1.7.2.1 Location

The IGCC plant is located at two facilities in Alberta, Canada: Suncor's Oil Sands processing (bitumen production and upgrading) facility located about 35 km north of the city of Fort McMurray and Suncor's Firebag lease located approximately 50 km northeast of the Oil Sands operation. The petroleum coke stockpile is located at the Oil Sands operation; therefore, equipment required for feedstock slurrying will be installed at the Oil Sands site. The resulting petroleum coke slurry will be sent via pipeline along the existing utility corridor between the two sites to the Firebag lease where the bulk of the IGCC plant is installed in order for the facility to be close to the steam injection point. (The engineering and cost for new pipelines (e.g. petroleum coke slurry and export streams) are outside the scope of this study).

The exact plot location of the gasification plant at the Firebag lease is to be determined; however, it is assumed that the plot is grubbed, level and free of any underground obstructions.

The following site data is based on information from Suncor and in-house Fluor information for the Suncor Oil Sands location. The elevation of the site at the Firebag Lease is approximately 550 meters above sea level with an average barometric pressure of 950 mbara. The maximum frost depth is 3.7 meters. Seismic design parameters (Z) are zero.

1.2.2.1.7.2.2 Meteorological Data

1.2.2.1.7.2.2.1 Site Temperatures

The site temperatures are summarized in Table 1.2.2.1.7.2.2.1(1).

Table 1.2.2.1.7.2.2.1(1) Site Temperatures, °C

Design (performance and plant size estimated at this temperature)	2.8
Average	2.8
Design maximum ambient dry bulb	35
Design minimum ambient dry bulb	-45
Design maximum ambient wet bulb	21.1
Maximum summer design*	28
Minimum winter design*	-40
Maximum recorded	36.1
Minimum recorded	-50.6

*Note: Normal process design: for critical services when the process is difficult to operate and/or control if the air temperature exceeds normal design air temperature for more than two hours, the maximum summer design is 31°C and the maximum winter design is –51°C.

1.2.2.1.7.2.2.2 Relative Humidity

The average relative humidity for the site is shown in Table 1.2.2.1.7.2.2.2(1).

Table 1.2.2.1.7.2.2.2(1) Relative Humidity, %

Design (performance and plant size estimated at this relative humidity)	68
Average	68
Minimum	50
Maximum	75

Note: No average relative humidity was available from site data; therefore, the average relative humidity was based on information from www.weatherbase.com for Fort McMurray, Canada.

1.2.2.1.7.2.2.3 Rainfall

Data for the site rainfall is shown in Table 1.2.2.1.7.2.2.3(1).

Table 1.2.2.1.7.2.2.3(1) Rainfall Data, mm

Maximum fifteen minute (10 year storm)	12
Maximum twenty four hour (10 year storm)	80

Annual average (including snow)	450

1.2.2.1.7.2.2.4 Snowfall

Data for the site snowfall is shown in Table 1.2.2.1.7.2.2.4(1)

Table 1.2.2.1.7.2.2.4(1) Snowfall Data

Ground snow load (S_s)	153 kg/m^2
Ground snow load (S_R)	10.2 kg/m^2
Maximum snow depth	1524 mm

1.2.2.1.7.2.2.5 Wind

Data for the site wind is shown in Table 1.2.2.1.7.2.2.5(1).

Table 1.2.2.1.7.2.2.5(1) Wind Data

Maximum wind velocity	20.1 m/s
Design wind speed	33.5 m/s
Average wind speed	4.5 m/s
Prevailing wind direction (summer)	North
Prevailing wind direction (winter)	South-East

Source: Fluor in-house data for TransAlta Energy Suncor Facility at Fort McMurray, Alberta.

1.2.2.1.7.3 Process Design Basis

1.2.2.1.7.3.1 Feedstocks

The Canadian Petroleum Coke Scenario is based on the gasification of petroleum coke. The amount of petroleum coke available for feedstock is not restricted and is set by producing 67,000 Nm^3/hr of hydrogen and fully loading the combustion turbines. The feed flow rate for the Advanced Case was set to be the same as that for the Controlled Baseline Case.

The analysis of the Suncor Oil Sands Petroleum Coke is shown in Table 1.2.2.1.7.3.1(1). All the data shown in the table are based on averages of test results performed on approximately 105 random samples taken from Suncor's petroleum coke stockpile. However, the Ultimate Analysis (average and range) is consistent with data used by ChevronTexaco to determine the performance of the Gasification Island.

Table 1.2.2.1.7.3.1(1) Petroleum Coke Analysis

	Average	Range	
As Received			
Moisture (weight percent)	10.0%	7.0%	11.3%
Air Dried			

Table 1.2.2.1.7.3.1(1) Petroleum Coke Analysis

	Average	Range	
Moisture (weight percent)	0.53%	0.31%	0.89%
Bulk Density (tonnes/m^3)	1.31	1.04	1.64
Hardgrove Grindability Index	47	40	55
Particle Size			
Less than 13 mm (½”)	77.8%		
Greater than 13 mm (½”)	22.2%		
Mineral Analysis (% weight in ash, air dried)			
SiO_2	44.70%	33.10%	63.54%
Al_2O_3	24.11%	10.77%	32.19%
TiO_2	3.29%	0.69%	9.66%
Fe_2O_3	9.11%	3.69%	14.96%
CaO_2	3.91%	1.15%	17.49%
V_2O_5	4.82%	1.46%	6.97%
Ni	0.93%	0.28%	1.58%
Dry Basis (weight percent)			
Volatile Matter	10.54%	9.28%	19.66%
Fixed Carbon	85.29%	74.67%	87.51%
Sulfur	5.91%	4.51%	7.11%
Ash	4.16%	2.57%	12.92%
Calorific Value, kJ/kg	33,540	30,670	34,471
(Btu/lb)	(14,420)	(13,186)	(14,820)
Ultimate Analysis (weight percent)			
Carbon	84.12%	83.18%	85.95%
Hydrogen	3.77%	2.95%	4.07%
Nitrogen	1.59%	1.12%	1.59%
Oxygen	0.26%	0.22%	1.80%
Sulfur	5.65%	4.51%	7.11%
Ash	4.61%	2.57%	12.92%