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A CALCIUM OXIDE SORBENT PROCESS
FOR BULK SEPARATION OF CARBON DIOXIDE

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EXECUTIVE SUMMARY

This research project is investigating the technical feasibility of a high-temperature, high-pressure (HTHP) process for the bulk separation of CO₂ from coal-derived gas. The original two-year contract was awarded in September 1989 as a result of solicitation number DE-RA21-89MC26040 entitled "Novel Concepts for Bulk Separation of Gases in Coal Gasification Systems". Two no-cost extensions without a change in the statement of work extended the performance period by six months to March 1992. At that time a two-year contract extension with an enlarged scope of work and additional funding was approved so that the contract now extends into March 1994.

The original Phase I project consisted of six tasks, with experimental work on five of the six completed prior to this reporting quarter. The latest extension, referred to as Phase II, added a seventh task to the project. The contents of this report are limited to a description of the final experimental results obtained in Phase I, Task 5, and a brief overview of the justification and plans for Phase II, Task 7.

TASK 5: MULTICYCLE TESTS

Initial tests in this task were completed prior to this quarter and those results were summarized in Annual Report 02. The primary objectives to be accomplished during the task were to extend the number of calcination/carbonation cycles to five (and to 10 in a few runs), and to examine sorbent reactivity and durability in gas compositions of increasing complexity. Those "on-matrix" tests which were carried out are identified in Table I by the run number in the appropriate matrix position. Runs which were completed prior to the beginning of this

Table I. Task 5 Five-Cycle Test Matrix.

SAMPLE	CALCIN PRESS (ATM)	CARBON TEMP. (C)	CARBONATION GAS COMPOSITION			
			A	B	C	D
7	1	750	(HP162)	-----	-----	-----
7	1	650	(HP157)	-----	-----	-----
7	15	750	(HP156)	HP206	HP221	HP230
7	15	650	(HP155)	HP209	HP220	-----
9	1	750	(HP161)	HP207	-----	-----
9	1	650	(HP163)	-----	-----	-----
9	15	750	(HP153)	HP205	HP218 HP225	HP226, HP229
9	15	650	(HP154)	HP208	HP219	-----

Carbonation Gas Composition:

A : 15%CO₂/N₂
 B : 15%CO₂/10%H₂O/N₂
 C : 5%CO₂/10%H₂O/5%CO/2.5%H₂/N₂
 D : 5%CO₂/10%H₂O/5%CO/2.5%H₂/0.22%H₂S/N₂

Calcination Condition:

Gas Atmosphere : N₂
 Temperature : 750 C

quarter are enclosed in parentheses while run numbers without parentheses represent data acquired during the present quarter. In addition, seven "off-matrix" tests which are identified in Table II were completed during the current quarter. The following discussion summarizes the results of all Task 6 tests.

Carbonation and calcination temperatures and pressures for the Task 6 tests were chosen on the basis of results from earlier tests. The purpose of the eight tests using carbonation Gas A (15% CO₂/N₂) was to determine if prior results obtained from two-cycle tests could be reasonably extrapolated to longer duration tests. Data from these five-cycles runs were characterized in terms of reactivity, R_i , and capacity C_i , with $i = 1, \dots, 5$. These results were presented in Annual Report 02 and will not be repeated here. Only the final conclusions will be reported.

1. Reactivity: The R_i values generally show a small decrease with increasing cycle number, and the magnitude of the decrease is somewhat larger for sorbent 7 than for sorbent 9. This result is in general agreement with the two-cycle test results. The only exceptions to the general trend of reactivity decrease occurred with sorbent 9 in the two tests using 750°C carbonation temperature. In both tests the reactivity exhibited a slight increase between cycles 1 and 2, followed by a reactivity decrease to the point that overall reactivity maintenance, R_{15} , was approximately 1.0. In the other six tests, the values of R_{15} were less than 1.0.

High carbonation temperature (750°C) produced higher values of the reactivity and reactivity maintenance indices for both sorbents. For example, using sorbent 9 with 15 atm calcination pressure, the values of

Table II. Task 5 Off-Matrix Multicycle Tests

Test No.

HP222	:	S-9 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, 5% CO ₂ /N ₂ , 15 atm (5 Cycles)
HP223	:	S-9 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, 7% CO ₂ /N ₂ , 15 atm (5 Cycles)
HP224	:	S-9 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, 5% CO ₂ /10% H ₂ O/N ₂ , 15 atm (5 Cycles)
HP227	:	S-9 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, 5% CO ₂ /10% H ₂ O/N ₂ , 15 atm (10 Cycles)
HP228	:	S-7 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, 5% CO ₂ /10% H ₂ O/N ₂ , 15 atm (10 Cycles)
HP231	:	S-9 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, gas C, 15 atm, 10 cycles (10 Cycles)
HP232	:	S-7 Calcination: 750°C, N ₂ , 15 atm Carbonation: 750°C, gas C, 15 atm, 10 cycles (10 Cycles)

R_1 at 750°C are, on the average, 30% greater than the R_1 values at 650°C. Similarly, $R_{15} = 1.02$ at 750°C compared to $R_{15} = 0.86$ at 650°C.

High calcination pressure (15 atm) had a moderately negative effect on R_1 for both sorbents at both carbonation temperatures. However, reactivity maintenance (R_{15}) was higher after high pressure calcination.

These five-cycle results were, in general, consistent with the earlier two-cycle results. Sorbent 7 was somewhat more reactive in the first cycle than sorbent 9 at all reaction conditions, but sorbent 9 exhibited better reactivity maintenance. Two-cycle results suggested that 750°C carbonation temperature was preferable, and this conclusion was substantiated by the five-cycle results. No previous results on the effect of calcination pressure were available, and the higher values of R_1 following one atmosphere calcination were somewhat surprising. Nevertheless, the improved reactivity maintenance at 15 atmospheres indicates that an isobaric calcination/carbonation cycle may, indeed, be feasible.

2. Capacity: Relatively little variation in first-cycle capacity was observed. The C_1 values for the eight tests using two sorbents, two calcination pressures, and two carbonation temperatures were all in the range of 0.94 to 0.98. C_1 values for sorbent 7 were slightly higher, ranging from 0.95 to 0.98, compared to 0.94 to 0.95 for sorbent 9. The capacity maintenance, however, was significantly better for sorbent 9, particularly at 750°C carbonation temperature. At 750°C carbonation temperature, $C_{15} = 0.98$ and 0.99 for the two sorbent 9 tests compared to $C_{15} = 0.89$ and 0.96 for the two sorbent 7 tests at the same conditions.

Higher carbonation temperature resulted in little change in C_1 for either sorbent. However, capacity maintenance was improved with 750°C carbonation temperature. The effect of calcination pressure on C_1 was

effectively negligible, but larger values of C_{15} were associated with 15 atm calcination. Overall the five-cycle capacity results were consistent with previous two-cycle results.

The remaining five-cycle tests shown in Table I were carried out to determine the effect of increasingly complex background gas compositions.

Gas B: The Effect of Steam

Five five-cycle tests were carried out using gas B composed of 15% CO_2 /10% $\text{H}_2\text{O}/\text{N}_2$. Earlier screening tests at one atmosphere under Task 2 suggested that H_2O might act as a promoter for the carbonation reaction. Since H_2O would be present in any coal gas, it was decided to examine any possible effects of H_2O before CO and H_2 were added to the reacting gas.

Severe experimental problems were experienced when steam was first added to the high-pressure carbonation gas. A typical electrobalance response during the carbonation cycle in a run in which 10% steam was introduced at 5 atmospheres is shown in Figure 1. For approximately 30 minutes, carbonation proceeded in a normal manner. Rapid initial carbonation was followed after approximately 5 minutes by the expected abrupt transition to the slow reaction phase. However, at 35 minutes an abrupt solid weight loss of about 4 mg occurred. Five minutes later another 4 mg of solid was lost. Two additional weight losses occurred before the run was terminated after 60 minutes. Only about 0.5 mg of solid remained in the sample pan. The actual solid loss was confirmed after the reactor was cooled and opened for inspection.

After much effort, the origin of the problem was determined to be condensation of steam on the inside of the reactor hang-down tube in the

Figure 1. Weight Loss Caused by Reactor Upsets During the Injection of Steam at High Pressure.

cool section where the hang-down tube joined the housing which contained the electrobalance mechanism. At elevated pressure the volumetric flow rate of inert gas through the housing was insufficient to prevent back-flow of reactive gas containing steam from reaching the cool surfaces. The problem was not encountered in the earlier atmospheric pressure screening tests because of the higher volumetric flow rate through the balance housing. Periodically, drops of condensate fell into the hot zone. Vaporization of the drops produced flow surges of sufficient intensity to dislodge portions of the sorbent from the sample pan.

In order to prevent steam from reaching the condensation surfaces, a stainless steel insert shown in Figure 2 was added to the upper section of the hang-down tube. The insert is supported by a press fit to the flange joining the balance housing and the hangdown tube. It is machined to provide a minimum gap between the insert and the hangdown tube. Near the bottom of the insert a teflon sleeve contacts the hangdown tube throughout its circumference to prevent steam from back diffusing to surfaces where condensation can occur. A small hole in the side of the insert provides for pressure equalization so that the teflon sleeve does not serve as a pressure seal. The insert terminates just above the side-arm where reactive gases are added. At the position of the teflon sleeve, the temperature is high enough to prevent condensation but low enough to avoid degrading the teflon. The reduced flow area of the insert provides sufficient velocity of inert gas from the balance housing to prevent steam from back diffusing up the insert and condensing there.

This insert eliminated the condensation problem and permitted the five-cycle runs using Gas B (Table I) to be completed without further

Figure 2. Diagram of the Insert Added to the Hangdown Tube to Prevent Steam Condensation.

problems. Problems of a different nature, not connected with steam condensation, were experienced when synthetic coal gas compositions were tested. These problems are described in the subsequent section.

Results of the five-cycle tests using gas B (containing 10% steam) confirmed the previous tentative findings that the presence of steam increased both the reactivity and capacity of the sorbents. These results are illustrated in Figures 3 and 4, where R_1 and C_1 are plotted versus cycle number for runs carried out at duplicate conditions except for the presence of steam in the carbonation gas.

In these figures, the times at which R_1 and C_1 have been evaluated have been shortened to 0.5 and 20 minutes, respectively. The previous reactivity comparisons were made at 1.0 minute and the previous capacity comparisons were made at 40 minutes. Because of the high CO_2 concentration used in all five-cycle runs (15 mol%) the fractional conversion after 1 minute was always quite large. The 1 minute comparison time for reactivity was chosen earlier as a compromise when the CO_2 mol fraction ranged from 0.01 to 0.15. $R_1(0.5)$ values are believed to provide a more reasonable basis for comparison at high CO_2 concentrations. The time for capacity comparisons was reduced from 40 to 20 minutes primarily as a matter of convenience. There is very little incremental sulfur sorption in the last 20 minutes, and reducing the carbonation cycle time is important in the long multi-cycle tests.

Figure 3 compares $R_1(0.5)$ and $C_1(20)$ values for two runs using sorbent 7 with calcination carried out at 15 atm and 750°C in N_2 , and carbonation at 15 atm and 650°C. Both the reactivity and capacity are significantly increased in run HF209 with steam in the carbonation gas. Similar results for sorbent 9 at the same reaction conditions are shown

Figure 3. Reactivity and Capacity Comparisons for Five-Cycle Tests With and Without Steam in the Carbonation Gas: Sorbent 7.

Figure 4. Reactivity and Capacity Comparisons for Five-Cycle Tests With and Without Steam in the Carbonation Gas: Sorbent 9.

in Figure 4. Both the reactivity and capacity are higher when steam is present in the carbonation gas.

Capacity maintenance also appears to be improved in the presence of steam. This is obvious in Figures 3 and 4 from the lower slopes of the $C_i(20)$ versus N curves for the runs containing steam. This result may be particularly significant since, in the gas A tests, 650°C carbonation temperature resulted in lower capacity maintenance than 750°C carbonation temperature.

Gas C: Simulated Coal Gas (Sulfur-Free)

Original plans called for the direct addition of 20% CO_2 and 10% H_2 to the gas B composition to produce a sulfur-free synthetic coal gas. The CO and H_2 were to replace N_2 . This planned composition was found to be unacceptable because of excessive carbon deposition on the walls of the reactor and the hangdown wire. The sorbent itself appeared to be free of carbon. Thermodynamic analysis of carbon deposition tendency predicted that the problem would be most severe as the reactive gas was heated to final reaction temperature, but less important once reaction temperature was reached. This was in agreement with the observed location of the carbon deposited in the reactor.

An alternate gas composition containing less carbon was then substituted with the original and substitute compositions shown below:

Composition (mol%)		
	Original	Substitute
CO_2	15	5
H_2O	10	10
CO	20	5

H ₂	10	2.5
N ₂	45	77.5

In the original gas the ratio of C/(O+H) was 0.438 while in the substitute gas C/(O+H) = 0.33. This change in composition did not completely eliminate carbon deposition, but reduced the quantity of carbon formed to a level small enough that it did not confound the kinetics results.

Four five-cycle runs using the substitute gas C were then carried out (see Table I). No adverse effects associated with CO and H₂ addition were noted. The stability of sorbent 9 in run HP218 is illustrated in Figure 5 where fractional carbonation is plotted versus time for each of the five cycles. For practical purposes the results for each cycle are identical.

Because of the lower CO₂ concentration in the substitute gas C (5%) it was not possible to make a direct comparison of results with gases A and B (15% CO₂). Therefore, a number of "off-matrix" five-cycle runs in which the carbonation gas contained 5 mol% CO₂ was carried out. These runs are designated HP222, HP224, HP227, and HP228 in Table II. An additional run containing 7% CO₂ was also carried out (Table II, run HP223). The significance of this run is described below

The addition of CO and H₂ to the carbonation gas created the possibility of the simultaneous occurrence of the water-gas shift and carbonation reactions:

While no direct confirmation of the simultaneous reactions is possible using the electrobalance reactor, our earlier one atmosphere screening tests had shown an increase in carbonation rate which would be

Figure 5. Time-Conversion Results for Five Carbonation Cycles of Sorbent 9 in Simulated Coal-Gas Atmosphere.

consistent with higher concentrations of CO_2 formed by water-gas shift. Shift equilibrium calculations using substitute gas C as the feed showed that approximately 7% CO_2 would be formed at equilibrium. This served as the justification for carrying out run HP223 using 7% CO_2/N_2 in the carbonation gas.

Fractional carbonation-time results for the first carbonation cycle for four tests are compared in Figure 6. The results of run HP222 where the carbonation gas consisted of 5% CO_2/N_2 are taken as the base case for the following comparison. Unexpectedly, the carbonation kinetics of the base run and HP223 (7% CO_2/N_2) are effectively the same. This lack of response to increased CO_2 concentration is not understood. Addition of 10% H_2O in run HP224 produced a clear increase in carbonation rate. This is consistent with the previously discussed direct promotional effect of H_2O on the carbonation rate. The highest overall carbonation rate was associated with test HP218 using gas C containing 5% $\text{CO}_2/10\%$ $\text{H}_2\text{O}/5\%$ $\text{CO}/2.5\%$ H_2/N_2 . The duration of the rapid initial reaction was also greatest for this test. Sorbent capacity, $C_1(20)$, is effectively the same in all four tests.

The increased reactivity of HP218 compared to HP224 is taken as further indirect evidence of the probable simultaneous occurrence of the carbonation and water-gas shift reactions. The presence of CO and H_2 in the HP218 carbonation gas provides all components necessary for the shift reaction to occur. This result is consistent with similar observations from the earlier Task 2 screening program.

Figure 6. First Cycle Carbonation Kinetics of Sorbent 9 In Different Gas Atmospheres.

Gas D: Simulated Coal Gas (With H_2S)

The final series of five-cycle tests were carried out with 0.22% H_2S added to gas C to produce a simulated coal gas containing sulfur. Three tests were carried out, although, for reasons to be described, the first test (HP226) was terminated after three cycles. As expected, H_2S reacted competitively with CO_2 , thereby reducing the carbonation capacity. In addition, the sulfidation reaction was irreversible so that, in a relatively short time, the entire sorbent was converted to CaS and no CO_2 removal was possible.

The effect of H_2S in the coal gas is most clearly shown in Figure 7 where normalized sorbent weight, W/W_0 , is plotted versus time for the three complete cycles of HP226. Zero time corresponds to the beginning of the first carbonation cycle, i.e., the sorbent had previously been calcined. During the early stages of the first carbonation cycle the sorbent weight increased rapidly due to the simultaneous reactions

A maximum value of $W/W_0 \sim 0.75$ was achieved after about three minutes. Thereafter, W/W_0 decreased due to the displacement of carbonate by the reaction

This reaction and the resultant sorbent weight loss continued until the reactive gas flow was stopped after about 30 minutes. In the 40 to 55 minute time period the remaining $CaCO_3$ was decomposed by calcination in N_2 . However, the final value of $W/W_0 \sim 0.58$ suggests that more than 50% of the calcium had been irreversibly converted to CaS during the first reaction cycle. The second carbonation cycle was initiated at 70 minutes and the maximum value of W/W_0 achieved was 0.68. The early

Figure 7. Weight-Time Response During Multicycle Carbonation of Sorbent 9 With H₂S in the Reacting Gas (Long Carbonation Cycle Time).

weight increase was again due to the simultaneous sulfidation and carbonation reactions. After reaching the maximum, W/W_0 decreased from 0.68 to 0.63, again due to the displacement of carbonate by sulfide. Third-cycle calcination in N_2 resulted in a reduction of W/W_0 to 0.61, which suggested that approximately 90% of the calcium had been converted to CaS. Very little weight gain occurred in the third carbonation/sulfidation cycle since only a small fraction of the calcium remained in the reactive CaO form. By the end of the third cycle, we estimated that about 98% of the calcium had been irreversibly converted to CaS.

Much of the loss of carbonation capacity in test HP226 was due to the replacement of carbonate by sulfur after the maximum value of W/W_0 was achieved. Consequently, in the subsequent test (HP229), the carbonation cycle was terminated just after the maximum weight was observed. Otherwise the reaction conditions in HP226 and HP229 were the same.

W/W_0 versus time results for five complete cycles of HP229 are shown in Figure 8. Although appreciate carbonation capacity was maintained throughout the five cycles, a continuing cycle-to-cycle decrease in capacity is evident due to the competitive formation of CaS. Figure 9 shows the increase in the estimated percent of calcium converted to CaS following each cycle for the two tests previously described as well as for an additional test (HP230), using sorbent 7, in which the time of the carbonation cycle was shortened as in test HP229. Sorbent 7 appeared to be even more susceptible to CaS formation than did sorbent 9. Even with the reduced carbonation cycle time, from 50 to 60% of the calcium was irreversibly converted to CaS after five cycles.

Figure 8. Weight-Time Response During Multicycle Carbonation of Sorbent 9 With H₂S in the Reacting Gas (Short Carbonation Cycle Time).

Figure 9. Build-Up of Calcium Sulfide During Multiple Carbonation Cycles.

It appears, therefore, that prior desulfurization will be required if the CaO sorbent is to be used for many cycles of CO₂ removal. However, it may still be possible to operate a "throw-away" process in which sorbent is rejected after being converted to CaS.

Ten-Cycle Test Results

The final four tests conducted in the Phase I portion of the program were extended to 10 complete cycles. Reaction conditions for these four tests (HP227, HP228, HP231 and HP232) are shown in Table II.

Figure 10 reports carbonation capacity, $C_i(20)$, versus cycle number for four tests using sorbent 7. Results from earlier five-cycle tests, HP206 and HP221, at the same conditions as HP228 and HP232, respectively, are included for comparison. In the simulated coal-gas atmosphere (gas C) the five-cycles results from HP221 match the ten-cycle results from HP232 quite well. The capacity decrease over the 10 cycles of HP232 was less than 10%. In the simpler test gas with no CO and H₂, sorbent performance during the ten cycle test (HP228) was considerably poorer than in the previous five cycle test at equivalent conditions (HP206). The first-cycle capacity of the two runs was essentially identical but HP228 suffered significant capacity loss in each subsequent cycle. Overall, for HP228 the capacity decreased by about 30% from the first to the tenth cycle.

Sorbent 9 has traditionally shown better capacity maintenance than sorbent 7 in short duration tests and this has been confirmed in the ten-cycle results. Figure 11 reports carbonation capacity, $C_i(20)$, versus cycle number for four tests using sorbent 9. The results from

Figure 10. Carbonation Capacity Versus Cycle Number for Ten Cycle Tests Using Sorbent 7.

Figure 11. Carbonation Capacity Versus Cycle Number for Ten Cycle Tests Using Sorbent 9.

two five-cycle and two ten-cycle tests at the same test conditions are shown. In this case, the results for all four tests are quite comparable, and in neither of the ten cycle tests is the capacity loss severe. In HP31 the capacity in the tenth cycle was only 1% lower in the tenth cycle than in the first cycle. In HP227 the capacity loss between the first and tenth cycles was approximately 3%. The capacity values for the thirty cycles represented by the four tests varied only between 0.93 and 0.97.

Further comparisons of multicycle stability are shown in Figures 12 and 13 where fractional carbonation-time results for the first, fifth, and tenth cycles of tests HP232 (Sorbent 7) and HP231 (Sorbent 9) are presented. Sorbent 7 (Figure 12) shows little change in initial reactivity, but the transition point between the rapid and slow reaction phases occurred at successively lower values of fractional carbonation as the number of cycles increased. This shift in the transition level prompted the decrease in capacity with increased cycle number. In contrast, the fractional conversion-time curves for each cycle for sorbent 9 (Figure 13) are essentially identical.

Summary

The experiments described above completed the experimental aspects of Phase I of the project. Extensive experimental data on the calcination and carbonation kinetics of three calcium-based sorbents was acquired as a function of calcination and carbonation temperature and pressure, CO_2 concentration in the carbonation gas, and background carbonation gas composition.

The three sorbents were obtained from precursors of different composition, and, as a result, the test sorbents exhibited a wide range

Figure 12. Time-Fractional Carbonation Results in the First, Fifth, and Tenth Carbonation Cycles: Sorbent 7.

Figure 13. Time-Fractional Carbonation Results in the First, Fifth, and Tenth Carbonation Cycles: Sorbent 9.

of surface area, pore volume, and pore size distribution. High pore volume was particularly important if high fractional calcium utilization was to be achieved during carbonation. Sorbents having high pore volume were obtained from precursors composed of hydrated calcium acetate (sorbent 7) and dolomite (sorbent 9). When a calcium carbonate precursor (sorbent 1) was tested, the calcined sorbent had low pore volume and low carbonation reactivity. While sorbents 7 and 9 exhibited similar first-cycle carbonation reactivity, the multicycle durability of sorbent 9 was clearly superior. This improved multicycle durability is attributed to a stabilizing effect of magnesium present in the dolomite precursor.

Reaction temperatures and background gas composition were found to be important reaction variables. Calcination temperatures in excess of 750°C caused the sorbent to sinter which resulted in a cumulative deterioration in performance during multicycle tests. The appropriate temperature window for the carbonation cycle was found to be in the 650-750°C range. Lower carbonation temperature (~550°C) produced an unexpected deterioration in sorbent performance over multiple cycles. No mechanistic explanation for the deterioration is available.

The addition of steam to the carbonation background gas produced an improvement in sorbent reactivity, capacity, and durability. Addition of CO and H₂ to produce a sulfur-free simulated coal-gas had no significant effect on the kinetics of the carbonation reaction. However, careful choice of gas composition was required in order to avoid carbon deposition in the reactor. Addition of H₂S caused a rapid and irreversible deterioration in carbonation capacity because of the irreversible reaction

In addition, H_2S was capable of displacing previously formed carbonate by the reaction

Since CaS(s) could not be reconverted to CaO(s) , a rapid and severe deterioration in carbonation capacity resulted. It appears, therefore, that a prior desulfurization step will be required before the calcium-based sorbent process can be used commercially for bulk separation of CO_2 .

Phase II Studies

The generally favorable results achieved during the Phase I studies justified an extension of the contract into Phase II work. The contract extension was approved in mid-March and only preliminary action has been initiated at this time.

The basic objective of the Phase II research is to scale-up the studies from the milligram quantities of sorbent used in the electrobalance studies to gram quantities of sorbent in a fixed-bed reactor configuration. The key analysis will shift from sorbent weight change monitored by the electrobalance to chromatographic analysis of the gas composition leaving the fixed-bed reactor as a function of time. This analytical capability will permit us to study both the primary CO_2 removal reaction

and the possible simultaneous occurrence of the water-gas shift reaction

If the water-gas shift reaction occurs either thermally

(noncatalytically) or if calcium and/or magnesium serves as a shift catalyst at reaction conditions, the possibility of a direct one-step process for the production of hydrogen from coal gas will be created. Production of H_2 by the shift reaction is normally equilibrium limited. However, in the presence of $CaO(s)$, CO_2 will be removed from the gas phase as it is formed thus permitting the shift reaction to continue producing $H_2(g)$.

The initial effort on the Phase II project consists of design and construction of the fixed-bed reactor coupled with acquisition of chromatograph system for product gas analysis. This effort is just getting underway at the end of the reporting quarter.

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