FOSSIL ENERGY

Advancement of Flash Hydrogasification Quarterly Technical Progress Report July-September 1984

By
A.Y. Falk

September 1985

Work Performed Under Contract No.: DE-AC21-78ET10328

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

By
Rockwell International
Rocketdyne Division
Canoga Park, California

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FOREWORD

This document is the third quarterly technical progress report summarizing work performed by Rockwell International for the U.S. Department of Energy, Morgantown Energy Technology Center (METC), under Contract DE-AC21-78ET10328* titled "Advancement of Flash Hydrogasification." The period of performance for the technical tasks of this contract work is from 23 December 1983 through 30 May 1985 (17 months). This report covers the period from 30 June 1984 through 28 September 1984.

The Rockwell program manager is Dr. Daniel R. Kahn. Technical administration of the program for DOE-METC is being provided by Mr. Gary R. Friggens.

*This basic contract has been modified several times since its inception in 1978. Formerly, it was referred to as "Coal Gasification Process Development" under DOE contracts ET-78-C-01-3125 and DE-AC01-78ET10328.

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The technical work on the Advancement of Flash Hydrogasification Program, Contract DE-AC21-78ET10328, is being organized and conducted under the technical direction of a Rockwell project engineer, Dr. Arthur Falk.

Major technical contributions to the conduct of the program during this report period were made by the following Rockwell personnel:

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Task VIII-B--Testing		V. Swanson
		M. Marko
Task VIII-C--Test Planning and Data Analysis		M. Schuman
		C. Erickson

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ABSTRACT

This third quarterly report documents technical progress during July through September 1984 on Rockwell International's Advancement of Flash Hydrogasification Program for the U.S. Department of Energy. The 17-month technical effort is divided into two major technical tasks: Task VII, Hardware Fabrication and PDU Modifications, and Task VIII, Performance Testing. The design of test hardware and process development unit (PDU) modifications had previously been completed as part of Task VI.

Task VII involves the fabrication of test hardware and the modification of an existing 1-ton/h hydroliquefaction PDU at Rockwell's facilities for use as a hydrogasifier test facility. Test hardware fabrication was completed in June 1984. During this report period, modifications to the PDU were completed in July, thereby ending the Task VII effort.

The modified facility is designed to accommodate both 10- and 20-ft-long hydrogasifier reactors so that residence times will be in the range of 2 to 6 s when coal is fed at a nominal 1/2 ton/h into reactors at 1000-psia pressure. Provisions have been made for real-time analysis of the product gases using an on-line gas chromatograph system. Separate supplies of coal, hydrogen, oxygen, methane, and water (for steam generation) are also provided. The facility and hardware changes now permit short-duration (1 to 2 h) hydrogasification tests and preburner assembly performance evaluation tests to be conducted to meet the test program objectives.

In Task VIII, test program planning and scheduling were approved by DOE in July, and programming of test data reduction programs was completed. During August, activation of the PDU was completed and testing was initiated. This involved conducting preburner performance characterization/checkout tests and the first two coal reactor tests. In general, the preburner assembly performed well and according to design; operation of the PDU has been smooth. Carbon conversions for the baseline (low steam concentration) coal hydrogasification tests were near predicted values.

I. INTRODUCTION

Under U.S. Department of Energy (DOE) sponsorship, Rockwell International has been developing a process for coal flash hydrolysis (FHP) based on the reaction of pulverized solid carbonaceous feedstocks with hydrogen at elevated temperature (1400 to 1900°F) in a single-stage, short-residence-time, entrained-flow reactor. Gases and liquids, if desired, are produced in the reactor, and unreacted material forms a dry, free-flowing char. Following product quench, liquid products are separated and gases are processed for recycle and product recovery. By varying the reactor operating conditions, the makeup of the product slate can be controlled over a broad range--from predominantly a syncrude oil with substitute natural gas (SNG) byproduct, to SNG with a relatively pure (>98 wt. %) benzene byproduct, to SNG alone as the sole hydrocarbon product. The hydrogasification process operates in one of the latter two product regimes, such that a large fraction of the feedstock's carbon is converted directly to methane.

On 10 May 1983, Rockwell initiated work on Task VI (Design of PDU Modifications) of the Coal Hydrogasification Process Development Program under DOE Contract DE-AC21-78ET10328. The objective of this task was to design the test hardware and facility modifications necessary to convert an existing 1-ton/h coal hydroliquefaction process development unit (PDU) at Rockwell's Santa Susana Field Laboratory for use as a hydrogasification test facility. This would provide the capability for subsequent engineering-scale testing to address key questions on reactor chemistry associated with the advancement of flash hydrogasification.

The Task VI design effort was conducted over a 5-month period ending in September 1983. The test hardware and facility modifications were designed such that the PDU would be capable of accommodating hydrogasifier testing over a wide range of operating conditions. The modified facility permits short-duration (1 to 2 h) hydrogasification testing and preburner performance evaluation testing to fulfill specific program objectives. Separate supplies of coal, hydrogen, oxygen, methane, carbon monoxide, and water (for steam generation) are provided for this purpose. The modified facility is designed to

accommodate both 10- and 20-ft-long hydrogasifier reactors so that residence times will be in the range of 2 to 6 s when coal is fed at a nominal 1/2 ton/h into reactors at 1000-psia pressure. Provisions have been made for real-time analysis of the product gases using an on-line gas chromatograph (GC) system.

A. PROGRAM OBJECTIVES

On 23 December 1983, DOE and Rockwell International mutually agreed to further amend the contract statement of work to incorporate two additional tasks: Task VII — Hardware Fabrication and PDU Modifications, and Task VIII — Performance Testing. The overall objective of the modified program is to investigate and verify the reactor chemistry associated with the Rockwell Advanced FHP concept for the production of SNG from coal. Specific objectives involve:

- Fabricating test hardware and modifying an existing 1-ton/h hydroliquefaction PDU to allow it to be operated in a mode that simulates the preferred reactor operating conditions.
- Operating the modified facility to develop the data base required to verify the reactor chemistry associated with the advancement of flash hydrogasification.

Further reflecting this modification of the scope of work, the contract title was changed to "Advancement of Flash Hydrogasification."

B. BACKGROUND

Rockwell International has been developing FHP of carbonaceous feedstocks under several DOE contracts since 1975. The basic Rockwell process concept and its flexibility in controlling the product slate are noted above.

A key element of the FHP reactor concept is the injector/reactor technology pioneered and developed by Rockwell. This technology, first used in liquid-fueled rocket engines, has several distinctive features that make it superior to alternative means of achieving the hydrolysis of carbonaceous

feedstocks. These include extremely rapid mixing and heating of reactants (10 to 20 ms), precise and uniform control of temperature and reaction time, rapid reactor startup and shutdown, unrestricted choice of feedstock, and simple scaleup. In addition, because the reactions occur in a short-residence-time (20 ms to 6 s), high-pressure (500 to 1500 psig), entrained-flow mode, the reactor is inherently compact. This permits shop fabrication of even commercial-scale hardware, with cost and reliability advantages over field fabrication. Reliability also benefits from the mechanically simple design and because it is economically possible to use high-quality materials in a more compact unit. The small reactor size contributes to rapid startup, stable operation, and facile process control. The small reactor size and modularity also make the process more readily maintainable than competitive processes and make incorporating a spare reactor cost effective. These factors lead to a projected increase in plant availability and thus benefit overall plant economics.

Rockwell International's first coal hydrogasification project, which began in March 1977 as a joint effort with Cities Service Company under DOE Contract EX-77-C-01-2518, involved a 20-month bench- and engineering-scale study.¹ Subsequently, Rockwell undertook the current development program under DOE Contract DE-AC01-78ET10328.

The initial engineering-scale hydrogasification tests conducted at Rockwell were performed in a 1/4-ton/h facility originally developed for hydroliquefaction testing. Forty-three successful tests were conducted, consisting of 30 tests with three types of coal (Montana Rosebud subbituminous, Kentucky hvAb, and Illinois hvCb) and 13 tests with Minnesota peat. Reactor pressures ranged from 500 to 1500 psig, temperatures from 1000 to 2000°F, and residence times from 500 to 5500 ms. Carbon conversions to gases as high as 71% with coal and 84% with peat were achieved. Tests were also run with hydrogen feed gases containing 15 to 20% CH₄, simulating a recycle process gas. After 1 year, testing was moved to a 1-ton/h PDU facility to allow running longer tests (1 to 2 h). Tests were conducted with the bituminous coals used in the smaller scale facility experiments.

At the conclusion of these test activities, the second contract²⁻⁴ was initiated. This effort consisted of testing in a 3/4-ton/h engineering-scale test unit (ETU), together with the design and construction of an 18-ton/day integrated process development unit (IPDU).

In the first year of testing under the second program, both Montana Rosebud subbituminous and Kentucky hvAb bituminous coals were used in the ETU. During the second year, 32 additional tests were completed, primarily with Kentucky No. 9 hvAb bituminous coal at a reactor pressure of 1000 psia. Injectors demonstrated stable operation with high carbon conversion to gas at low hydrogen-to-coal ratios (0.2 to 0.4 by weight). A hydrogen-cooled recuperator was constructed and tested. Significantly, three replicate runs (tests 318-36, -37, and -50) were made under nearly identical conditions and produced results showing high reproducibility. This demonstrated the advance of the hydrogasification process to the stage of reliable test operations. These runs also demonstrated a high carbon conversion to BTX (~11%) and subsequently served as the design point for a commercial plant design performed by the Lummus Company under subcontract to Rockwell. The BTX (benzene-toluene-xylene) produced from the reactor is 98 to 99% benzene and can be readily upgraded to chemical-grade purity using existing commercial technology.

Design of the IPDU facility was completed in May 1980, and construction at Rockwell's Santa Susana Field Laboratory near Los Angeles proceeded until being halted by DOE at about 60% completion. The facility is designed for continuous operation for periods up to 30 days and has provisions for on-site coal storage, coal pulverization and drying, pneumatic lock hopper pressurization of the pulverized coal feed, lock hopper letdown of the char produced, and work-around (versus remote) facility operation.

Rockwell has also performed extensive modeling studies and has developed a sophisticated coal FHP reactor model for correlation and prediction of FHP hydrogasification and hydroliquefaction test results. The method used involved

defining a set of phenomenological reactions representing the processes occurring during FHP and then applying a nonlinear multiple regression technique to a set of equations derived according to the kinetics of those reactions.⁴

As an integral part of Rockwell's Coal Hydrogasification Process Development Program, the Lummus Company (now Lummus Crest, Inc.), with the concurrence of DOE, prepared under subcontract to Rockwell a preliminary design of a complete 250 billion Btu/day commercial-scale SNG-from-coal plant based on the Rockwell Coal Hydrogasification Process. This 18-month study culminated in the issuance of a predesign report, submitted to Rockwell in May 1981, entitled "Coal Hydrogasification Plant--Preliminary Design Study for a 250 Billion Btu-Per-Day SNG Plant."⁵ In addition to the 250 billion Btu/day of SNG, the baseline plant was designed to produce 5310 bbl/day of chemical-grade benzene as a coproduct. The plant showed excellent economic potential: using the economic methodology developed by C. F. Braun⁶ for DOE, Lummus estimated the cost of gas at \$3.68 per million Btu in mid-1979 dollars. Total plant investment was estimated at \$1331 million, including a 15% project contingency.

Beyond the DOE-sponsored programs, Rockwell has continued its efforts to advance FHP technology and has studied process alternatives with potential for improving the process, increasing its efficiency, reducing capital requirements and operating costs, etc. These in-house Rockwell studies have been aimed primarily at alleviating the expensive burden of makeup hydrogen production, freeing the process from dependence on other developmental technologies, and simplifying downstream product processing. These efforts yielded a new Rockwell process concept--termed Advanced FHP.

A Rockwell coal FHP reactor model was used extensively in developing the Advanced FHP process. This model enabled coal conversion levels and reactor effluent compositions to be predicted as functions of reactor operating conditions. Combining these results with parallel analyses of downstream processing led to the establishment of desired process operating points. Various process designs were subsequently developed and their economics evaluated. This Rockwell process design effort provided the basis for further proposed

experimental testing and led to the present modification of Contract DE-AC21-78ET10328 to investigate and verify the reactor chemistry associated with the Advanced FHP concept.

II. SUMMARY OF PROGRESS DURING QUARTER

A schedule for the Advancement of Flash Hydrogasification Program is presented in Figure 1. The 17-month technical effort is divided into two major tasks: Task VII, Hardware Fabrication and PDU Modifications, and Task VIII, Performance Testing.

Task VII is divided into three subtasks: Task VII-A, Test Hardware Fabrication; Task VII-B, Facility Modifications; and Task VII-C, Process Systems Modifications.

Test hardware fabrication and facility modifications were completed during the previous report period. Work on the process systems modifications ended in July 1984 to complete the Task VII effort.

Task VIII is divided into three subtasks: Task VIII-A, System Activation; Task VIII-B, Testing; and Task VIII-C, Test Planning and Data Analysis.

The test program plan and schedule was approved by DOE in July 1984; system activation was completed in late August 1984; and testing is now in progress. Preburner performance characterization/checkout testing and two coal reactor tests at baseline hydrogasification conditions have been successfully completed to date. The preburner assembly performed well and according to design. For the coal reactor tests, carbon conversions were near predicted values, and operation of the PDU was generally smooth.

During startup for the third reactor test on 28 September 1984, a small localized burnout occurred in the inside wall of the water-cooled preburner assembly combustion chamber. This problem has been attributed to high wall heat fluxes near the preburner injector and the inadvertent use of "hard" coolant water. Resolution of the problem is in progress. It is estimated that about a 3-week delay in testing will occur. Testing is currently about 1-month behind schedule, and is expected to extend through January 1985.

MAJOR MILESTONE LOG

▲ 1 FACILITY MODIFICATIONS COMPLETED

▲ 2 TEST HARDWARE FABRICATION COMPLETED

▲ 3 PROCESS SYSTEMS MODIFICATIONS COMPLETED

▲ 4 FACILITY ACTIVATION INITIATED

▲ 5 FACILITY ACTIVATION COMPLETED

▲ 6 REACTOR TESTING INITIATED

▲ 7 REACTOR TESTING COMPLETED

▲ 8 DATA ANALYSIS COMPLETED

▲ 9 DRAFT TOPICAL (TASK VIII) AND FINAL REPORTS SUBMITTED

▲ 10 APPROVED TOPICAL (TASK VIII) AND FINAL REPORTS SUBMITTED

◆ DRAFT

□ FINAL

28 SEPTEMBER 1984

Figure 1. Advancement of Flash Hydrogasification Program Schedule

III. DISCUSSION OF PROGRESS DURING QUARTER

The technical effort on DOE Contract DE-AC21-78ET10328, Advancement of Flash Hydrogasification, was initiated on 23 December 1983. This third quarterly technical progress report summarizes work performed between 30 June 1984 and 28 September 1984. The program is divided into two major tasks, each containing three subtasks, as noted below:

Task VII--Hardware Fabrication and PDU Modifications

- Task VII-A--Test Hardware Fabrication
- Task VII-B--Facility Modifications
- Task VII-C--Process Systems Modifications

Task VIII--Performance Testing

- Task VIII-A--System Activation
- Task VIII-B--Testing
- Task VIII-C--Test Planning and Data Analysis

During this report period, work was continued on Tasks VII-C, VIII-A, and VIII-C. Task VIII-B was initiated in late August 1984. Progress on these various tasks is discussed in detail below.

A. TASK VII--HARDWARE FABRICATION AND PDU MODIFICATIONS

Tasks VII-A and VII-B were completed in June 1984. Detailed descriptions of the test hardware and facility modifications were presented in the two previous quarterly technical progress reports^{7,8} and hence will not be repeated here.

1. Task VII-C--Process Systems Modifications

The design of the process system modifications required to convert the 1-ton/h hydroliquefaction PDU for use in flash hydrogasification was completed as part of Task VI of this contract. The schedule of activities and the status of the modifications to the process systems are summarized in Figure 2.

Figure 2. Status of Process System Modifications (Task VII-C)

This task includes: (1) preparation of the PDU for subsequent subcontractor facility modifications (Task VII-B); (2) system component procurement and servicing; (3) detailed layout and installation of the instrumentation, controls, and data acquisition system (DAS); (4) updating of system test procedures; (5) installation and/or modification of various feed systems; (6) installation of an on-line GC sampling system; and (7) assembly and installation of the reactor train into the PDU.

During this report period, the test system instrumentation, controls, and DAS were installed in the PDU facility, and the test hardware was inserted into the reactor pressure vessel. Installation of the carbon monoxide gaseous feed system had originally been postponed pending results of the preburner performance testing. Successful high conversion of methane to carbon oxides in the preburner testing did, however, make it unnecessary to install the carbon monoxide system. The process system modifications effort was completed in late July 1984.

The process system modifications are described in detail in the two previous quarterly technical progress reports^{7,8} and will not be repeated here.

B. TASK VIII--PERFORMANCE TESTING

All of the Task VIII subtasks were active during this report period. System activation (VIII-A) was completed in late August 1984, Testing (VIII-B) was initiated during the last week of August 1984, and Test Planning and Data Analysis (VIII-C) continued as planned. The status of activity on these tasks is discussed separately below.

1. Task VIII-A--System Activation

Activation of the test system was initiated during June 1984 in conjunction with the process system modifications. This effort included (1) checking out the instrumentation and control wiring, (2) installing instrumentation

transducers onto the PDU, (3) programming the DAS, (4) activating the GC analyzers and sampling system, and (5) activating all feed and product recovery systems. System activation was completed during the third week of August, about 1 month behind the original program schedule.

2. Task VIII-B--Testing

The test program plan presented in the last quarterly technical progress report⁸ was approved by DOE on 25 July. The major objectives of the test program are as follows:

- Check out the operation and performance of the preburner and steam generator subsystems.
- Determine baseline product slates under hydrogasification conditions at high reactor exit temperatures and long residence times.
- Determine the extent to which steam in the reactor reacts with char to produce carbon oxides. Similarly, determine whether steam affects the hydrocracking of vapor-phase liquid hydrocarbons.
- Determine the effects of temperature and injected reactor gas composition on the product slate.
- Determine the effects of carbon oxides generated in the preburner system by partial oxidation of methane on the reactor chemistry and product slate.
- Acquire credible material balances and obtain quantitative data on the coal elemental conversions and the slate of hydrocarbon products obtained under suitable FHP reactor conditions.

Testing began on 28 August 1984, with the first of five preburner assembly tests. Five preburner and two reactor tests were successfully completed during this report period. The preburner and reactor test durations are summarized in Table 1.

TABLE 1
SUMMARY OF PREBURNER AND REACTOR TEST DURATIONS

Test Number	Date	Number of Test Conditions	Duration ^a (min)
PB-1A	28 Aug 84	1	22
PB-1B	30 Aug 84 (a.m.)	5	47
PB-1B	30 Aug 84 (p.m.)	2	37
PB-1C	05 Sep 84	3	68
PB-2	07 Sep 84	3	84
R-1	19 Sep 84	1	92 (52)
R-2	24 Sep 84	1	70 (52)
R-3A	28 Sep 84	-	8

^aO₂ flow time to preburner. Value in parentheses for tests R-1 and R-2 are coal flow times.

Operation and performance of the preburner assembly was characterized over a wide range of operating conditions encompassing 14 test conditions and 4-1/2 h of operation. The two reactor tests, each about 1 h in duration, were conducted to check out the facility and establish performance at low inlet steam concentration to the FHP reactor. Results of these reactor tests will provide a baseline for defining steam enhancement on subsequent reactor tests.

During startup for the third reactor test on 28 September 1984, the preburner combustion chamber was damaged. This happened before the start of coal flow, and the system was shut down by an automatic "cut" sequence initiated by the DAS when low preburner coolant water flow was detected. Post-test hardware inspection revealed a small localized burn-through in the water-cooled preburner combustion chamber inside wall near the preburner injector. The preburner combustion chamber pressure is higher than the coolant water system pressure. Consequently, the wall burn-through allowed combustion gases to pass through the hole in the inside chamber wall and into the coolant water

passage. This gas flow restricted the flow of coolant water, resulting in the test "cut" sequence. Test R-3 was designed as a high reactor exit temperature (~2000°F) and high steam concentration (~45%) test to investigate steam enhancement effects. Preburner operating conditions were similar to those successfully employed during preburner test PB-1C.

After preliminary analysis, the test hardware problem was attributed to high chamber wall heat fluxes near the preburner injector and the inadvertent use of "hard" coolant water. Resolution of this problem, which involves increased cooling of the chamber wall near the injector, is in progress. Additional wall cooling will be provided by decreasing the inside chamber wall thickness, increasing the coolant water velocity, and reversing the coolant water flow direction in order to supply lower-temperature, higher-pressure water to the high heat flux region. The water conditioning unit that supplies the "soft" coolant water will be monitored for proper operation on each filling of the coolant water supply tank. It is estimated that about a 3-week delay in testing will occur as a result of implementing the above changes.

a. Preburner Performance Characterization/Checkout Testing

The main objective of these tests was to check out the operability and performance of the preburner assembly. These tests also served as checkouts for the on-line GC system and provided experience in controlling critical system temperatures and flow rates. No coal was fed to the FHP reactor during these tests.

Test Planning - Testing was intended to cover a range of conditions that spanned the preburner assembly operating conditions planned during reactor testing. The operating conditions targeted for the preburner performance characterization/checkout tests are presented in Table 2. The expected main injector exit gas composition, assuming 100% conversion of methane to CO in the preburner assembly, is also noted.

TABLE 2
TARGET TEST CONDITIONS FOR PREBURNER PERFORMANCE CHARACTERIZATION/CHECKOUT TESTS^a

Test	Test Condition	H ₂ /CH ₄ /O ₂ Preburner				Steam Generator			Main Injector				
		Flow Rate (lb/h)			Exit Temperature ^b (°F)	Flow Rate (lb/h)		Exit Temperature ^b (°F)	O ₂ Flow Rate (lb/h)	Exit Temperature ^b (°F)	Exit Gas Composition (mole %)		
		H ₂	CH ₄	O ₂		H ₂ O	H ₂				H ₂	Steam	CO
PB-1	1	168	0	172	2500	0	154	1200	86	1600	89.9	10.1	0
PB-1	2	168	0	237	3000	0	154	1500	86	1900	87.3	12.7	0
PB-1	3	168	0	237	3000	0	250	1200	187	1900	87.2	12.8	0
PB-1	4	168	0	309	3500	0	250	1500	110	1900	87.1	12.9	0
PB-1	5	212	0	297	3045	543	138	1200	195	1900	70.1	29.9	0
PB-1	6	212	0	377	3500	543	138	1500	118	1900	70.0	30.0	0
PB-1	7	256	0	446	3500	1043	48	1500	126	1900	55.2	44.8	0
PB-2	8	172	80	440	3500	447	150	1500	138	1900	69.5	28.0	2.5
PB-2	9	172	140	531	3500	723	97	1500	138	1900	59.2	36.6	4.4
PB-2	10	128	269	659	3500	781	86	1500	138	1900	53.1	38.5	8.4

^aH₂/CH₄ inlet temperature = 1100°F; H₂O inlet temperature to steam generator = 200°F; inlet temperature of all other reactants = 70°F.

^bCalculated exit temperatures include estimated test hardware heat losses.

The purpose of test PB-1 (no methane addition) was to provide information on the preburner and main injector H_2/O_2 ignition characteristics, system heat losses, and preburner assembly steam generation capability. This was accomplished by successively increasing the $H_2/CH_4/O_2$ preburner exit temperature from approximately 2500 to 3500°F at 1200 and 1500°F steam generator exit temperatures. The main injector exit temperature was limited to a maximum of 1900°F, and sufficient spray quench water was injected at the reactor exit to cool the reactor products to 850°F. Initial testing was performed without adding water to the steam generator. The sequence of tests was set up for ease of transition to increasingly more severe test conditions. Sufficient time was planned at each test condition to verify steady-state conditions, as indicated by on-line GC analyses and steady flow rates and temperatures.

Test PB-2 involved methane addition to the preburner, and the planned conditions shown in Table 2 cover a range typical of that required for subsequent coal testing with methane addition. From this test, the percentage of methane conversion and the corresponding gas compositions at various conditions were defined.

With the exception of the main injector exit temperature, which may be greater than 1900°F during the reactor tests (by the addition of more O_2 to the main injector), the test conditions in Table 2 are intended to simulate the full range of desired reactor test conditions.

Test Results - Actual test conditions for the preburner performance characterization/checkout tests are presented in Table 3. Tests PB-1A and PB-1B were conducted to define the system performance without hot water injection for steam generation. The steam generation capability of the preburner assembly was demonstrated during test PB-1C. The main injector exit gas composition was measured by on-line GC at a point about 6 in. from the main injector face. The measured values were in close agreement with theoretically derived values as shown in Table 3 for Tests PB-1C and PB-2.

TABLE 3
ACTUAL TEST CONDITIONS FOR PREBURNER PERFORMANCE CHARACTERIZATION/CHECKOUT TESTS

Test Number	Test Condition	H ₂ /CH ₄ /O ₂ Preburner				Steam Generator			Main Injector							
		Flow Rate (lb/h)			Exit Temperature ^a (°F)	Flow Rate (lb/h)		Exit Temperature (°F)	O ₂ Flow Rate (lb/h)	Exit Temperature (°F)	Exit Gas Composition ^b (mole %)					% CH ₄ Conversion to CO _x
		H ₂	CH ₄	O ₂		H ₂ O	H ₂				H ₂	Steam	CO	CO ₂	CH ₄	
PB-1A	1	166	0	177	2497	0	153	1268	68	1561						
PB-1B	2	169	0	182	2480	0	152	1264	0	1192						
PB-1B	3	169	0	182	2485	0	151	1268	65	1544						
PB-1B	4	167	0	236	2917	0	150	1506	66	1766						
PB-1B	5	166	0	229	2877	0	251	1152	67	1381						
PB-1B	6	166	0	229	2877	0	245	1169	156	1729						
PB-1B	7	170	0	306	3397	0	250	1429	0	1364						
PB-1B	8	168	0	301	3382	0	249	1411	100	1746						
PB-1C	9	212	0	291	2897	454	118	1333	129	1773	74.5 (72.9)	25.0 (27.1)				
PB-1C	10	207	0	340	3237	525	120	1440	115	1799	71.8 (70.1)	28.1 (29.9)				
PB-1C	11	238	0	395	3308	913	49	1414	122	1790	59.4 (57.3)	40.1 (42.7)				
PB-2	12	169	80	356	2940	434	147	1249	0	1192	75.8 (76.3)	21.5 (21.1)	2.15 (2.55)	0.2	0.3	90
PB-2	13	167	78	427	3415	443	150	1471	88	1737	73.2 (71.3)	24.1 (26.2)	2.16 (2.46)	0.04	0.05	98
PB-2	14	168	48	527	3365	694	92	1483	85	1737	63.4 (60.9)	31.1 (34.4)	4.50 (4.70)	0.7	0.2	96

^aCalculated (complete conversion of CH₄ to CO assumed for CH₄ addition tests).

^bValues in parentheses are theoretical for test conditions. Tests with methane addition assume complete conversion of CH₄ to CO.

During test PB-2, the capability of the $H_2/CH_4/O_2$ preburner to convert methane to CO_x (primarily CO) was demonstrated. As expected, methane conversion to CO_x increased with increasing $H_2/CH_4/O_2$ preburner exit temperature, from 90% at 3000°F to 98% at 3500°F. The composition of the commercial-grade methane fed to the system during test PB-2 is given below in Table 4. The high conversion of methane to CO_x in the preburner eliminates the need for the gaseous CO feed system during subsequent coal reactor tests.

TABLE 4
COMPOSITION OF COMMERCIAL-GRADE
METHANE FED TO PREBURNER ASSEMBLY

Component	Composition (mole %)
Methane (CH_4)	93.7
C_2H_6	3.2
C_3 's	0.8
CO_2	0.7
N_2	1.6

Figures 3 and 4 present DAS-generated plots of selected system temperatures and flow rates as a function of time during test PB-1A. The preburner assembly exit temperature and system hydrogen and oxygen flow rates are shown in Figure 3. The initial temperature rise is due to heating the preburner hydrogen flow in the facility hydrogen heater. An abrupt decrease in the preburner assembly exit temperature is noted when the ambient temperature steam generator hydrogen flow is initiated. The sudden increase in temperature observed when the preburner oxygen flow was started indicates H_2/O_2 ignition in the preburner. Oxygen flow to the preburner was turned on when the injection temperature of the preburner hydrogen (not shown in Figure 3) reached about 1200°F.

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Figure 3. Preburner Assembly Exit Temperature and Flow Rates
as a Function of Time During Preburner Test PB-1A

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Figure 4. Selected System Temperatures as a Function of Time During Preburner Test PB-1A

Figure 4 presents selected system temperature plots. Note the abrupt increase in reactor gas temperatures with main burner ignition (start of main burner O_2 flow). In general, system flow rates and critical temperatures were easily controlled at desired values. Control of critical system pressures, although not shown in Figures 3 or 4, was also quite good.

In summary, the completed preburner performance characterization testing was very successful. The following goals were achieved:

- Operability and performance were demonstrated, including:
 - . Reliable preburner and main burner ignition
 - . Successful steam generation
 - . High conversion of CH_4 to CO_x
 - . Total preburner assembly heat loads near predicted values
- System control and operating characteristics were defined, resulting in:
 - . Smooth, easily controllable operation over desired operating range
 - . Successful checkout of gas feed and product systems and on-line GC system.

b. Reactor Testing

The reactor testing phase of the program began on 19 September 1985 with coal test R-1. The objectives of the first two reactor tests were to check out the PDU facilities involving the coal feed system and to establish baseline hydrogasification carbon conversions at long residence times and high reactor exit gas temperatures. For these tests, no methane or hot water for steam generation was added to the preburner. The steam concentration of the injected gas was maintained at the system's minimum value (13 to 15%). Only the steam generated from the addition of oxygen to heat the hydrogen to its required injected temperature was fed to the reactor.

Nominal reactor conditions for the first two tests were 1000-psig reactor pressure, 5-s residence time, 0.2 reactor inlet gas-to-coal (moles/lb) ratio, an inlet gas composition of ~14% steam and 86% H₂, and 60 min in test duration. The reactor exit temperatures for tests R-1 and R-2 were targeted at ~1800 and 2000°F, respectively.

Actual test conditions for the first two reactor tests are summarized in Table 5, while reactor inlet and exit gas compositions are presented in Table 6. The solids feedstock to the reactor was a Kentucky No. 9 high-volatile A bituminous coal pulverized to approximately 90% < 200 mesh. Detailed properties of the coal, including proximate and ultimate analyses, free swelling index, ash fusion temperature in a reducing atmosphere, and sieve analysis, are provided in Table 7.

TABLE 5
TEST CONDITIONS FOR REACTOR TESTS

Test Number	R-1	R-2
Date	19 Sep 84	19 Sep 84
Reactor pressure (psig)	1000	1000
Injected gas temperature (°F)	2014	2116
Reactor exit temperature (°F)	1845	1982
Residence time (s)	5.2	5.0
Test duration (min)	52	52
System flow rates (lb/h)		
Coal	927	958
Preburner H ₂	175	170
Preburner CH ₄	0	0
Preburner O ₂	303	305
Steam generator H ₂ O	0	0
Steam generator H ₂	226	232
Main injector O ₂	129	154
Reactor inlet gas-to-coal ratio (moles/lb)	0.22	0.21

TABLE 6
REACTOR INLET AND EXIT GAS COMPOSITION FOR REACTOR TESTS

Test Number	R-1	R-2
Inlet gas composition (mole %)		
H ₂	86.6	85.6
Steam	13.4	14.4
Exit gas composition (mole %)		
H ₂	73.6	69.4
Steam	14.0	14.6
CH ₄	11.3	14.4
C ₂ H ₆	T ^a	T
C ₆ H ₆	0.19	ND ^b
CO	0.81	1.47
CO ₂	0.10	0.13

^aTrace (<0.02%)

^bND (Not Detected)

Plots of key system temperatures and flows as a function of time are presented in Figures 5 through 8 for the two reactor tests. System startup before the start of coal flow is similar to that of the preburner tests described earlier. The dynamic nature of the hot gas/coal mixing can be seen by the fluctuations in the reactor inlet temperature. This parameter is measured by a thermocouple located in the flow stream just 6 in. downstream from the injector face. In general, system flows, temperatures, and pressures (not shown in Figure 5) were fairly steady during the coal flow period. The main burner oxygen flow rate was increased slightly approximately 8 min after the start of coal flow during test R-2 to increase the reactor exit temperature to its desired value (Figure 7). The reactor product stream was quenched to about 850°F at the reactor exit and further cooled to near ambient temperature in the light oil condenser.

The exothermic nature of the hydrogasification reactions is evidenced by the approximately 250°F increase in temperature over the length of the reactor

TABLE 7

PROPERTIES OF KENTUCKY NO. 9 HIGH-VOLATILE A BITUMINOUS COAL^a

1. Proximate analysis, as received ^b		Moisture (%)	2.10
		Ash (%)	8.20
		Volatile (%)	40.46
		Fixed carbon (%)	49.24
		Sulfur (%)	2.96
		Btu/lb	13,254
2. Ultimate analysis, dry basis ^b		Carbon (%)	74.09
		Hydrogen (%)	5.15
		Nitrogen (%)	1.49
		Chlorine (%)	0.09
		Sulfur (%)	3.02
(by difference)		Ash (%)	8.38
		Oxygen (%)	7.78
3. Free swelling index ^b			5-1/2
4. Fusion temperature of ash (reducing) ^b		Initial deformation (°F)	2070
		Softening (H = W) (°F)	2185
		Softening (H = 1/2 W)	2300
		Fluid (°F)	2410
5. Sieve analysis ^c	U.S. Sieve Series Number	Sieve Opening (μm)	Cumulative Amount Passing Through Sieve (wt. %)
	400	37	11.8
	325	44	19.1
	200	74	86.8
	100	149	98.6
	50	297	99.6
	30	595	100.0

^aProvidence Mine No. 1^bAnalysis by Commercial Testing & Engineering Company (Lombard, Illinois)^cAnalysis by Rockwell

Figure 5. Reactor Inlet Temperature and Hydrogen and Oxygen Flow Rates as Functions of Time for Test R-1

Figure 6. Selected System Temperatures as Functions of Time for Test R-1

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Figure 7. Reactor Inlet Temperature and Hydrogen and Oxygen Flow Rates as Functions of Time for Test R-2

Figure 8. Selected System Temperatures as Functions of Time for Test R-2

(inlet versus exit temperatures in Figures 6 and 8). This temperature rise along the reactor is further illustrated in Figure 9, wherein reactor wall temperature is shown plotted as a function of reactor length for both reactor tests. The reactor wall temperatures were measured on the outside wall of the thin reactor tube. Note that the temperature rise occurs much faster at the high-temperature reactor conditions (test R-2).

Carbon conversions based on measured gas and benzene production and as-collected carbon, hydrogen, and ash balances for the reactor tests are summarized in Tables 8 and 9, respectively. Several discrepancies were observed in the data from the first reactor test. The ash balance was higher (~115%) and the overall conversion was considerably lower than that predicted by Rockwell's FHP coal reactor model.⁴ An overall carbon conversion of near 57% was predicted for test R-1 based on the FHP model.

TABLE 8
CARBON CONVERSIONS FOR REACTOR TESTS

Test Number	Carbon Conversion (%)						
	Overall ^a	To Char ^b	CH ₄	C ₂ H ₆	C ₆ H ₆	CO	CO ₂
R-1	50.8	49.2	42.2	0.13	4.9	3.1	0.38
R-2	58.0	42.0	51.8	0.07	-	5.7	0.51

^aBased on measured gases plus benzene

^b100 minus overall

TABLE 9
CARBON, HYDROGEN, AND ASH BALANCES
FOR REACTOR TESTS

Test Number	As-Collected Balances		
	Carbon	Hydrogen	Ash
R-1	94.4	104.4	115.4
R-2	98.3	108.5	100.9

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Figure 9. Reactor Wall Temperature Profiles for Tests R-1 and R-2

The as-collected (measured) balances in Table 9 represent the portion of each component exiting the system relative to the quantity entering in the various feed streams. The method used to calculate these values was described in the data analysis plan presented in the last quarterly technical progress report.⁸ To substantiate the accuracy of the gas flow rate measurements, hydrogen throughput flow checks were conducted in conjunction with each reactor test. For these flow checks, steady test values of preburner and steam generator hydrogen flows were established, and inlet and exit flow rates were then measured in the normal fashion (i.e., with NBS traceable, calibrated venturi meters). The inlet and outlet gas flow checks were in good agreement for both tests.

The abnormally high ash balance on test R-1 has been attributed to residual oil shale char remaining in the system from previous oil shale FHP testing. The last test program completed in the PDU used an Eastern oil shale as feedstock. Eastern oil shale char contains about 5% carbon and 90% ash; whereas typical Kentucky No. 9 coal gasification chars contain approximately 70% carbon and 20% ash. It was estimated that only ~0.6 gal of residual oil shale char would be required to account for the high ash balance on test R-1. The reason for the high hydrogen balances is still being investigated.

Overall carbon conversions calculated by requiring an ash balance were 60.3 and 59.8% for tests R-1 and R-2, respectively. The large discrepancy between overall conversion based on an ash balance and that based on the measured gas plus benzene production (Table 8) is partially attributable to contamination from the residual oil shale char, as noted above. However, the residual oil shale char would have a negligible effect on the carbon balance because of its low carbon content. Overall carbon conversion calculated from the carbon remaining in the char was calculated for each test. On this basis, the resulting overall carbon conversions for tests R-1 and R-2 were 56.4 and 59.7%, respectively. These latter values of overall carbon conversion are more reasonable and consistent. Corresponding carbon conversions to char would therefore be 43.6 and 40.3% for tests R-1 and R-2, respectively.

Carbon conversions predicted from Rockwell's FHP coal reaction model versus those experimentally determined are presented in Table 10. The experimental values for overall, char, methane, and CO_x are near the nominal predicted values. However, the experimental benzene conversions are substantially below the model's predictions. The experimental data suggest that about 5% of the coal carbon may have been converted to unrecovered light oil during test R-1, since overall carbon conversion minus the carbon conversion to gases plus benzene is about 5%, and the carbon balance is also about 5% low. The differences between the model's predictions and experimental carbon conversions are most likely due to the fact that the model is based primarily on data at shorter residence times and lower temperatures. Presently, the high temperatures and long residence times of tests R-1 and R-2 are extrapolations of the model. As further data are generated on this program, the model will be updated accordingly.

TABLE 10
COMPARISON OF PREDICTED AND EXPERIMENTAL CARBON
CONVERSIONS FOR REACTOR TESTS

Test Number	Carbon Conversion (%)				
	Overall	To Char	CH_4	C_6H_6	CO_x
R-1					
Predicted	57	43	43	9	4.5
Experimental	56.4	43.6	42.2	4.9	3.5
R-2					
Predicted	62	38	53	4.5	4.5
Experimental	59.7	40.3	51.8	-	6.2

Based on the results of the first two reactor tests, the following can be concluded: (1) the main injector and reactor are operating as designed; (2) PDU operation has been smooth; (3) excellent control of test conditions can be obtained; (4) the on-line GC is performing well; and (5) good carbon, hydrogen, and ash balances can be achieved in the PDU test system.

In the next coal reactor test (R-3), the effect of steam enhancement will be investigated. For this purpose, test conditions will be run at a high steam concentration (~45%) and high reactor exit temperature (~2000°F).

c. Preburner Hardware Burnout

As discussed earlier, during startup for the third reactor test on 28 September 1984, a small localized burnout occurred in the inside wall of the water-cooled preburner combustion chamber. Preliminary analysis indicates that the actual heat fluxes near the preburner injector were several times greater than those originally estimated during hardware design (Task VI). Further, it was found that the soft water system employed for cooling the preburner chamber assembly was not operational. Repeated usage of hard water could cause the buildup of scaly deposits on this key cooling surface and significantly reduce the heat transfer in the hot region of the preburner combustion chamber.

Resolution of this problem is now in progress. This will involve providing for increased cooling of the chamber wall near the preburner injector, and restoring to full operation the soft water cooling system. It is estimated that about a 3-week delay in testing will occur as a result of the hardware repair activities.

d. Test Schedule

Figure 10 presents the current Task VIII-B test schedule. As indicated above, the first 3 weeks in October will be required to repair the preburner combustion chamber damage. Thereafter, testing will resume on an estimated one-test-per-week basis through January 1985. Two 1-week hiatus periods in testing are also planned, one for installation of the shorter-residence-time reactor and one for the year-end holidays. Up to 15 reactor tests are scheduled to be performed in Task VIII-B.

TEST SERIES	TEST NUMBER	1984																1985					
		SEPTEMBER				OCTOBER					NOVEMBER				DECEMBER			JANUARY					
		PROJECT WEEK																					
		37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58
A	PB-1/PB-2	1	2																				
A	R-1, R-2, AND R-3			1	2			3															
B	R-4 THROUGH R-9									4	5	6	7	8	9								
—	INSTALL SHORTER RESIDENCE-TIME REACTOR																						
B	R-10 THROUGH R-15																						

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Figure 10. Current Schedule for Testing (Task VIII-B)

3. Task VIII-C--Test Planning and Data Analysis

During July, the test program plan and schedule were approved by DOE, and the programming of test data reduction programs was finalized. The status of the Task VIII-C effort is summarized in Figure 11. Current activity involves the analysis of the test data, which will continue approximately 1 month beyond the last reactor test.

▼ TEST PROGRAM PLAN AND SCHEDULE SUBMITTED TO DOE

Figure 11. Test Planning and Data Analysis Status (Task VIII-C)

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