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THE MIXING AND GASIFICATION OF COAL IN ENTRAINED FLOW SYSTEMS

Quarterly Technical Progress Report
for the Period 1 January, 1976 to 31 March, 1976

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This report summarizes technical progress accomplished during the fifth report period of a two-year study being conducted for the Energy Research and Development Administration (ERDA) under contract No. E(49-18)-1767. This work period was 1 January 1976 to 31 March 1976. Work was accomplished under the direction of Dr. L. Douglas Smoot, principal investigator and Dr. Richard W. Hanks, senior investigator. Dr. Paul Scott is the technical representative for ERDA.

Graduate and undergraduate students who have contributed to the technical progress and to this document were James Barnett, Stanley Harding, Vincent Memmott, Brent Montague, Dee Rees, Jerry Sharp, Douglas Skinner, Christopher Tice, and Scott Woodfield. Mr. James Hoen, Supervisor of the Research Machine Shop, is providing assistance in reactor design and construction, while Dr. Ralph L. Coates has served as an advisor. Michael King, Karen Weis and Scott Folster have provided technician, typing, and drafting services.

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ABSTRACT

This report presents work accomplished during the fifth quarter to investigate mixing and gasification of coal in entrained flow systems. Visits to Washington State University, Arizona University and ERDA were made during the report period.

Design of the major gasifier components was completed with final drawings, and fabrication of inlet components, reactor feeder and scrubber was initiated. Secondary preheater and steam generator were ordered and delivery dates were set. A "critical-path" schedule for gasifier design, fabrication and installation was developed. Particle size variation of the test coal was measured.

Ten non-reacting, non-recirculating jet mixing tests were conducted using test conditions similar to coal gasifiers. Results show particle dispersion much slower than gas mixing. Particles also seemed to retard gas mixing. Extension of this facility to permit recirculating tests was continued.

Programming of the macroscopic, coal gasifier model was nearly completed and sample input data were prepared for initial trial computer runs. Plans for the next quarter include completion of fabrication and start of assembly of gasifier components, performance of several non-reacting jet mixing tests, and debugging of the macroscopic gasifier model.

OBJECTIVE AND SCOPE OF WORK

Background

Two national goals of great importance to every citizen of the United States are the development of adequate energy supplies and the establishment of a satisfactory living environment. Vast domestic reserves of coal cannot presently be used directly without degrading the environment beyond the limits specified by current environmental quality laws. As a consequence, conversion of this fossil fuel into a more desirable form is an intermediate solution to the problem of meeting energy demands.

As attempts have been made to produce large, clean, economical supplies of gas and oil from coal, a number of different types of coal gasification processes have been proposed, explored, and developed. Several of these coal gasification processes involve, either directly or indirectly, the injection of finely powdered coal, suspended in a gas stream, into a reactor where the conversion reactions take place, creating a variety of different products. Associated with such entrained particle processes are technological problems involving the entrainment of the coal. The basic principles of this process are not well understood and require considerable study before optimal engineering designs are possible. One problem associated with the entrainment of the coal particles is the influence of the turbulent mixing characteristics of a particle-laden gas stream, the resultant rates of chemical reactions which take place in the reactor, and the subsequent yield of products. Such mixing problems have been identified (1) as among the most critical and key problems which need to be solved in order to improve the design of entrained gas reactors. While some work has been and is being conducted (2, 3) to determine the effects of mixing on the kinetics of direct combustion of pulverized coal, very little work has been reported which deals with the basic processes of coal gasification. The present study deals specifically with the influences of turbulent mixing on coal gasification processes.

Objectives

The general objective of this research program is to develop an understanding of physical and chemical rate processes that occur during gasification of entrained, pulverized coal particles. Specific tasks that have been outlined for accomplishment during the first phase of this study are:

1. Conduct visits to facilities where research and development on entrained coal gasification units are in progress. Identify more specifically the configurations, operating conditions, and input properties of reactants and clarify the nature of potential particle/gas mixing problems.

2. Analyze in detail the configurations, reactant systems, and operating properties in entrained coal gasifiers and char combustors and select a set of variables for a subsequent experimental test program. Variables to be considered will include: (1) operating conditions, such as pressure, residence time and flow rates; (2) configurations, such as injection angle and reactor size; (3) reactant stream conditions, such as temperature, gas phase composition, particle size and particle loading level.

3. Design and construct a laboratory-scale test facility, capable of operation over a range of conditions for study of non-reacting and reacting coal/char/gas systems in different geometries. Include the capability to sample the particle/gas mixtures locally in order to determine the extent of gas mixing, the extent of particle dispersion, the amount of particle reaction, and the local product composition.

4. Conduct a series of non-reacting tests using the laboratory scale facility to determine the gas dispersion rates and recirculation effects for various operating conditions, stream compositions, and geometric configurations.

5. Interpret experimental particle/gas dispersion results and analyze for potential impact on configuration and operating conditions in entrained coal-gasification units.

6. Initiate the development of a computerized mathematical model for describing reacting coal gasification and char combustion processes.

This first phase of this work has been scheduled to be accomplished in a two-year study period. The second phase of the program will emphasize reacting coal gasification tests and comparison of measurements with model predictions.

Technical Approach

In order to accomplish the tasks outlined above, two entrained flow reactors are being designed and constructed. One reactor will operate at atmospheric pressure while the second reactor will be designed to operate at a peak pressure of 20 atm.

The atmospheric reactor is being constructed principally to study direct coal combustion using funds from a separate project supported by EPRI (3). However, this reactor will also have the capability to gasify coal and combust char at atmospheric pressures. The high pressure reactor, which will require a longer period to design, construct and evaluate, is being developed principally to study entrained coal gasification processes at elevated pressures, and is being constructed using funds from this study. The high pressure reactor will have a primary nozzle diameter of 1.27 cm, and will have a coal processing capacity of 13.6-136 kg/hr.

A third test facility to study mixing processes of non-reacting flows is already available at this laboratory and is being used for this project to study mixing of non-reacting, particle-laden flows at atmospheric pressure conditions.

Experimental plans for Phase I require two separate sets of non-reacting tests: (1) A series of non-reacting, atmospheric tests using the existing atmospheric, non-reactive test facility. (2) A series of non-reacting, high-pressure tests using the reactive high pressure test facility being designed as a part of this study. It is also planned that reactive coal gasification checkout tests for atmospheric and higher pressure will be conducted toward the end of this first phase of study. Additional information concerning the basic approach was outlined in the first quarterly progress report (4).

SUMMARY OF PROGRESS TO DATE

Figure 1 shows a summary chart of research activities by task. Progress to date in each of the tasks is summarized below.

Task 1. Facility Visits. Facility visits have been completed. This task included visits with Bureau of Mines, BCRI, Koppers Corporation, Babcock and Wilcox, Foster and Wheeler, and Combustion Engineering in the United States. International Flame Foundation, Cherchar, Bergbau Forschung, BCURA, CERL, National Coal Board Labs and British Gas Corporation facilities were visited in Europe. Contact and interchange is being maintained with U.S. companies.

Task 2. Variable Selection. Development of the test variables and tentative test programs have also been completed and were reported in detail in the first and second quarterly progress reports (4, 5). For non-reactive tests, two series of tests (with and without recirculation), have been outlined for several different test conditions. Test variables include primary velocity (15, 30 m/sec), secondary velocity (30, 60 m/sec), percent solids in primary stream (40, 60%), injection angle (0, 30 degrees), secondary/primary density (0.1, 0.47), aft-duct diameter (13-35 cm), and particle size (30, 70μ).

Development of test conditions and test programs have also been completed for the entrained gasification tests. Coal feed rate will be about 140 kg/hr. Variables will include pressure (1-20 atm), coal type, injection angle (0, 30 degrees), secondary preheat temperature (315, 430°C), secondary velocity (15, 25 m/sec), solids loading level (70-80%), and coal size. The tentative test program includes 54 tests.

Task 3. Facility Design and Construction. During the past quarter, design of the major high pressure facility components was completed and all working drawings were prepared for items requiring fabrication.

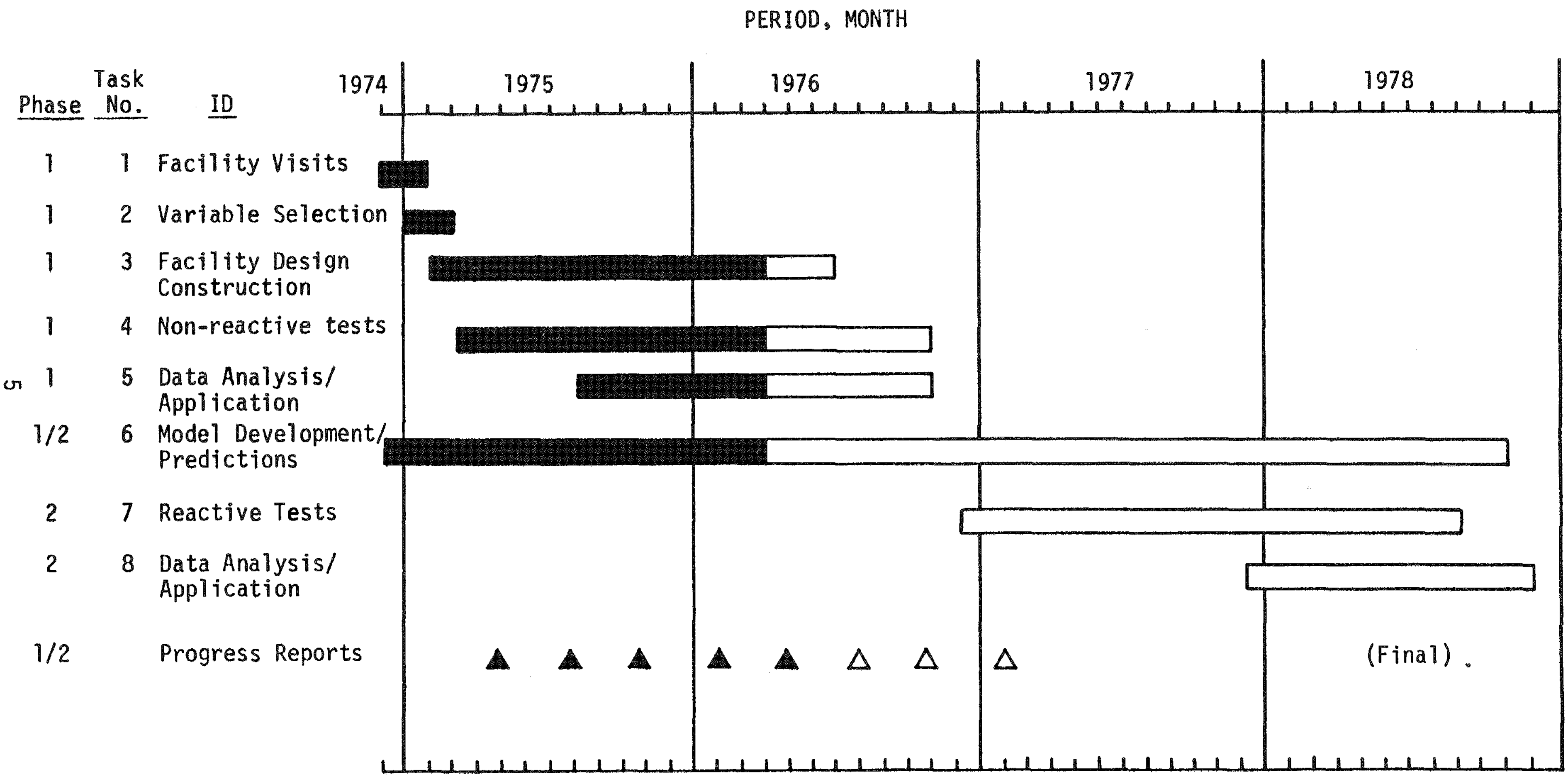

Figure 1. Summary Chart of Research Activities

Fabrication of primary/secondary inlet components was partly completed and reactor fabrication was initiated. Fabrication of the scrubber and feeder were nearly completed by an outside shop. The secondary preheater and steam generator were ordered and delivery dates set. Designs of the ignition system and probe system were initiated. Variation in pulverized test coal particle size was determined. A study was initiated to determine possible measurement of pollutants.

Task 4. Non-Reactive Tests. Ten tests were conducted for non-recirculating flows, including 4 checkout tests and 6 final data tests. Modification of the facility for subsequent recirculating tests was continued.

Task 5. Data Analysis. The computer program for data reduction was reviewed and revised for these tests. Data for the non-reacting tests were analyzed. Test symmetry and material balance accuracy were very good. Results show significant influences of injection angle. Particles disperse more slowly than gases and also influence gas mixing.

Task 6. Model Development. An iterative computer solution scheme was developed for the macroscopic coal gasification model. Most of the solution programming was completed and a sample input problem was prepared. Plans were made for initial computer debugg runs.

Progress Reports. To date, five quarterly progress reports and an annual summary report have been prepared and submitted to ERDA. In addition, a summary paper of study results has been presented at a technical conference and the follow-on proposal for phase 2 has been submitted.

DETAILED DESCRIPTION OF TECHNICAL PROGRESS

Technical Visits and Reviews

During January of this report period, L. Douglas Smoot visited Washington State University (WSU) and discussed a possible cooperative research program related to modelling of entrained gasifiers. Dr. David Pratt, Dr. Clayton Crowe, Dr. Stephen Schmidt, and Mr. John Wormack, from WSU participated in these discussions. Subsequently, during February, Pratt and Smoot visited Dr. Paul Scott of ERDA/Washington, D.C. to discuss further a proposed program addition for the gasifier model development.

Technical discussions were also held during the report period with Dr. J.O.L. Wendt and Mr. David Pershing of Arizona University regarding coal combustion characteristics.

Technical literature review during this report period has emphasized coal pyrolysis. References reviewed and analyzed included Anthony, et al. (6) and Field, et al. (7).

Non-reacting Tests

The objective of the atmospheric, non-reacting tests is to measure rates of turbulent mixing of particle-laden jets with and without recirculation for test conditions typical of pulverized coal combustors and gasifiers. Initial non-reacting tests are being conducted using an existing test facility (8).

Without Recirculation. A revised test schedule for the non-reactive tests has been outlined as summarized in Table 1. These test conditions correlate with the typical test conditions for coal combustion and gasification. Final testing has been initiated according to this test program. Silicon powder (41μ mass mean diameter) was selected for the non-reacting tests because of its similarity to coal in density, while being available as spherical particles of controlled size ranges. Size characteristics of the unclassified silicon have been analyzed and are compared with those of the pulverized bituminous coal to be used in the reacting tests as shown in Table 2. Tests will be conducted with this unclassified silicon and also with various cuts of this powder where particle size is more nearly constant.

Ten tests were completed during this period with the revised facility. These tests are summarized in Table 3. The first four tests were primarily to check out the revised facility. The last six tests were part of the final test program. Radial argon composition profiles at 0.18 m and 0.31 m from the exit plane from two of the six tests are illustrated in Figure 2. The silicon powder mass flux curve at 0.31 m is shown in Figure 3. Similar profiles are obtained in each test. The results of these tests show excellent symmetry in the collection of both the gas and the silicon powder. These results also show that the primary gases are mixing much more rapidly with the secondary air than are the particles.

Figure 4 shows a plot of new centerline concentration data for test condition I for the powder and argon from all 6 final tests and compares these results with parallel flow data from Fejer (9). While additional tests are to be performed for this test condition, several interesting observations are shown. Firstly, mixing of the powder and the gases is much faster with injection of the secondary air at 30°, as shown by comparing lines A, B, C with line D. Secondly, the particles disperse much more slowly than the gases, as shown by comparing lines A and B with line C. Finally, it appears that the presence of the particles is retarding the mixing of the gases, as shown by comparing lines A and B. This last observation is based on too little data to be conclusive.

These data being obtained for non-reacting flows will show the effects of test conditions, injection angle and particle concentration on rates of jet mixing and will also provide a basis for evaluating predictive models.

With Recirculation. The components of the recirculating facility are completed with the exception of the probes for the probe collar. These

TABLE 1

SUMMARY OF REVISED TEST CONDITIONS FOR

NON-REACTING, NON-RECIRCULATING TESTS

Test ID	I		II		III		IV		V		VI	
Parameter	Pri	Sec	Pri	Sec	Pri	Sec	Pri	Sec	Pri	Sec	Pri	Sec
Velocity, ft/sec	100	125	100	125	100	200	100	125	100	125	100	125
Temperature, °F	50	50	50	50	50	50	50	200	50	50	50	50
Pressure, psia	13.0	13.0	13.0	13.0	13.0	13.0	13.0	13.0	13.0	13.0	13.0	13.0
Particle size	std.		std.		std.		std.		small		large	
Flow Rate, g/sec												
Air	5.4	456	5.4	456	5.4	729	5.4	564	5.4	456	5.4	456
Argon	17.4	--	17.4	--	17.4	--	17.4	--	17.4	--	17.4	--
Particles	15.2	--	34.2	--	15.2	--	15.2	--	15.2	--	15.2	--
% Solid Loading	40.0	--	60.0	--	40.0	--	40.0	--	40.0	--	40.0	--
% Mole Argon	70.0	--	70.0	--	70.0	--	70.0	--	70.0	--	70.0	--
Sec/Pri												
Velocity	1.3	--	1.3	--	2.0	--	1.3	--	1.3	--	1.3	--
Gas Density	0.8	--	0.8	--	0.8	--	0.6	--	0.8	--	0.8	--
Total Density	0.47	--	0.32	--	0.47	--	0.1	--	0.47	--	0.47	--
Gas Flow	20.0	--	20.0	--	32.0	--	15.5	--	20.0	--	20.0	--
Total Flow	12.0	--	8.0	--	19.2	--	9.3	--	12.0	--	12.0	--
Injection Angles	--	0-30	--	0-30	--	0-30	--	0-30	--	0-30	--	0-30

[1]std = unclassified, as received silicon

TABLE 2

SIZE CHARACTERISTICS OF COAL AND SILICON

A. Bituminous Coal

Arithmetic Average Size of Increment (microns)	Weight % in Increment		Mass Mean Diameter (microns)	Specific Surface Area cm^2/gm
5.70	0.00	0.00		
7.20	0.00	0.00		
9.00	0.01	0.01		
11.40	0.02	0.02		
14.35	0.06	0.06		
18.10	0.16	0.15		
22.80	0.43	0.40	58.8[1]	377
28.70	1.06	0.98		
36.15	2.44	2.27		
45.55	5.49	5.11		
57.40	13.0	12.1		
72.30	29.3	27.2		
91.10	48.1	44.7	sieve cut line	
127.0		5.00		
179.0		1.70	74.7[2]	265
210+		0.30		

ρ = 2.26 gm/cc

B. Silicon

Arithmetic Average Size of Increment (microns)	Weight % in Increment	Mass Mean Diameter (microns)	Specific Surface Area cm^2/gm
5.70	0.00		
7.20	0.01		
9.00	0.04		
11.40	0.11		
14.35	0.27		
18.10	0.72	40.9	505
22.80	1.91		
28.70	4.95		
36.15	11.89		
45.55	18.40		
57.40	20.76		
72.30	29.87		
91.10	11.07		

ρ = 2.33 gm/cc

1. Mean diameter of smaller cut only
2. Mean diameter of entire mixture

TABLE 3

SUMMARY OF TESTS COMPLETED DURING REPORT PERIOD

Test No.	Condition*	Injection Angle	Probe Axial Location(m)	Test Comments
1	I	30°	0.18	Symmetry check-out test
2	I	30	0.18	Gas only-good symmetry
3	I	30	0.31	Gas only-excellent symmetry
4	I	30	0.31	35μ Si powder excellent symmetry
5	I	30	0.31	35μ Si powder excellent symmetry
6	I	30	0.31	Standard Si powder excellent symmetry
7	I	30	0.11	Standard Si powder excellent symmetry no gas analysis
8	I	30	0.11	Standard Si powder excellent symmetry gas analysis problems
9	I	30	0.18	Standard Si powder excellent symmetry gas analysis problems
10	I	30	0.56	Standard Si powder No gas analysis

*See Table 1 for a detailed description of the test condition.

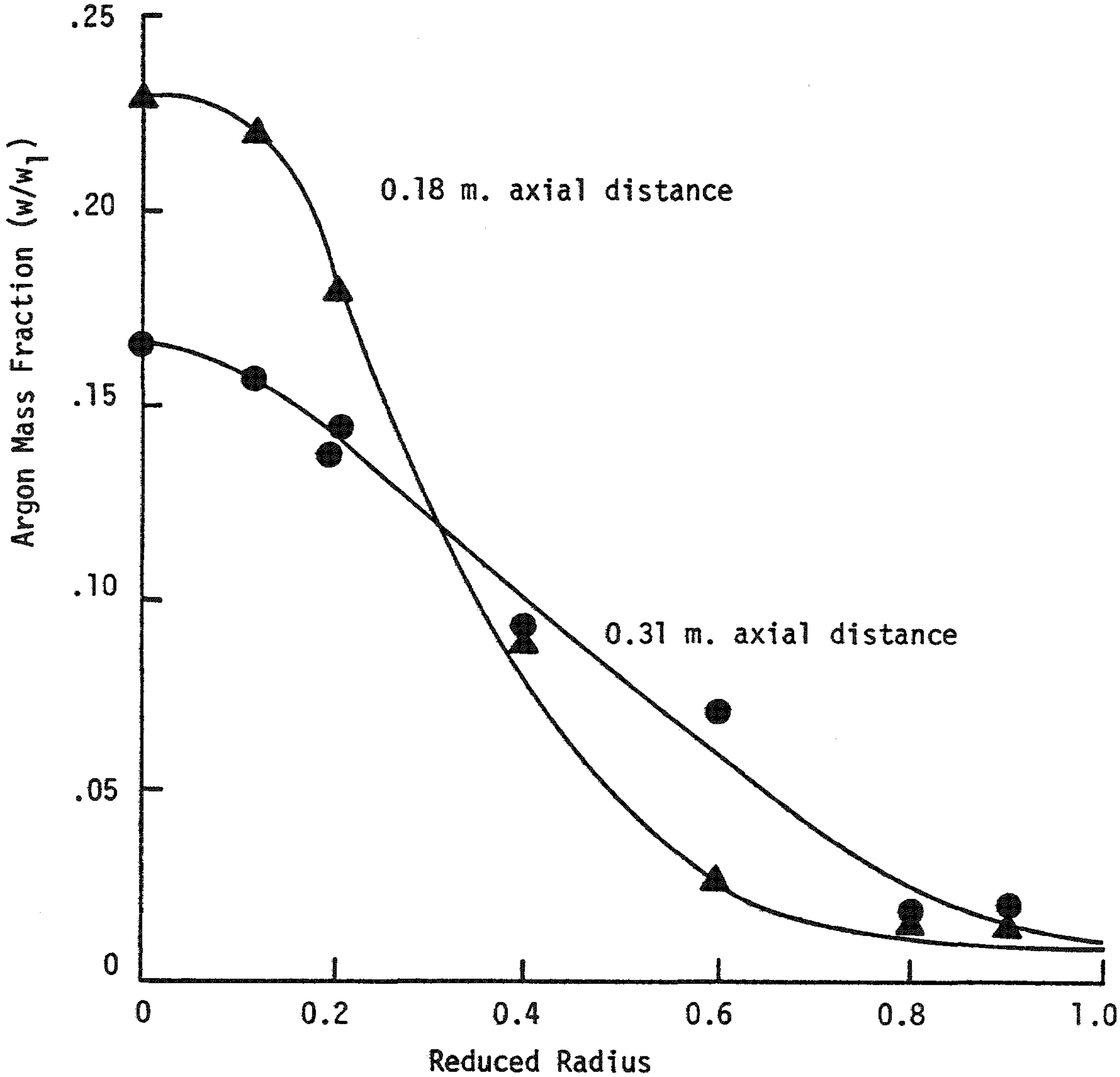

Figure 2. Argon Radial Profiles (Test Condition I, 30° injection).

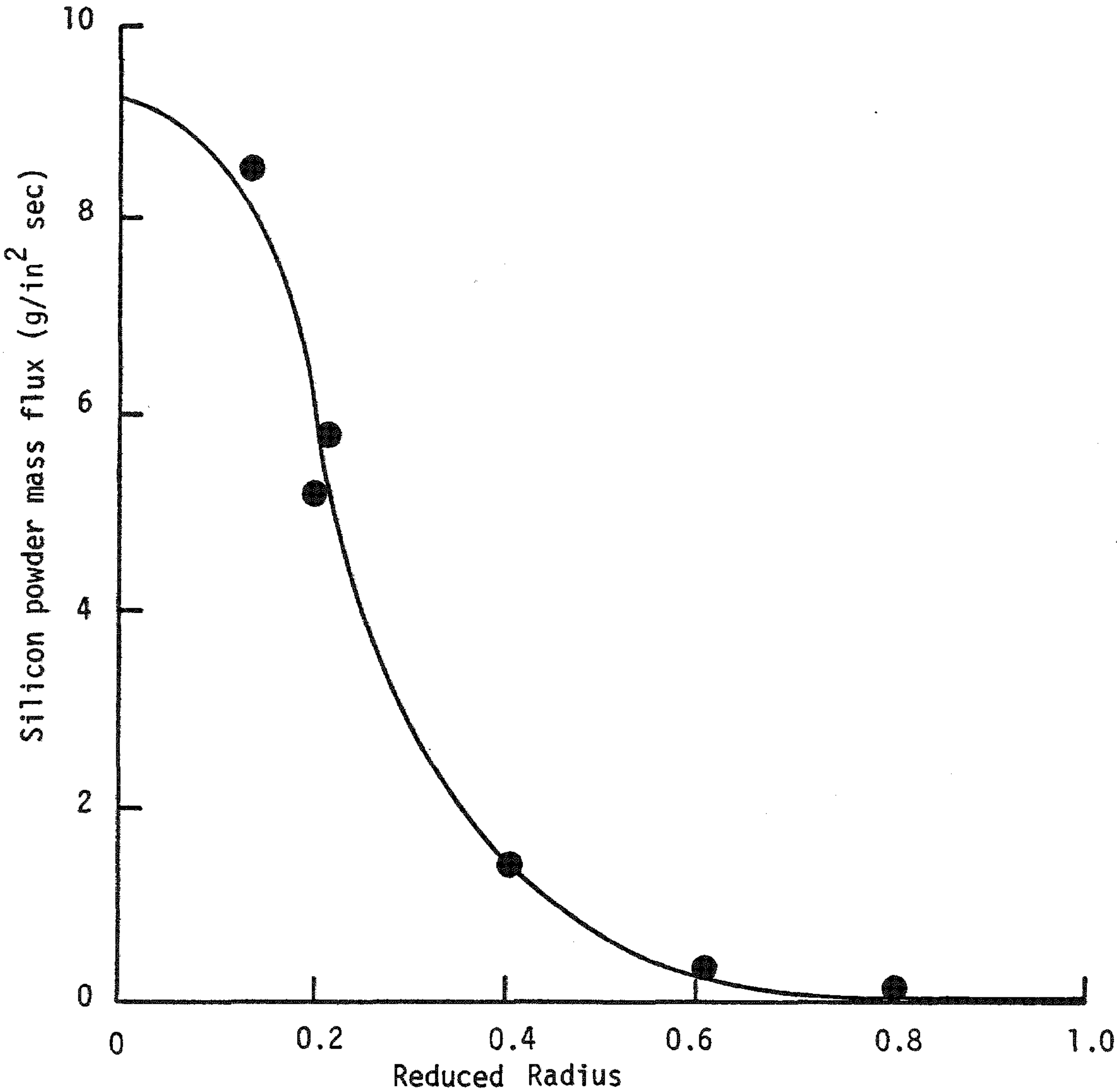

Figure 3. Silicon Particle Radial Profile (Test Condition I, 30° injection, 0.31m. aft of exit plane).

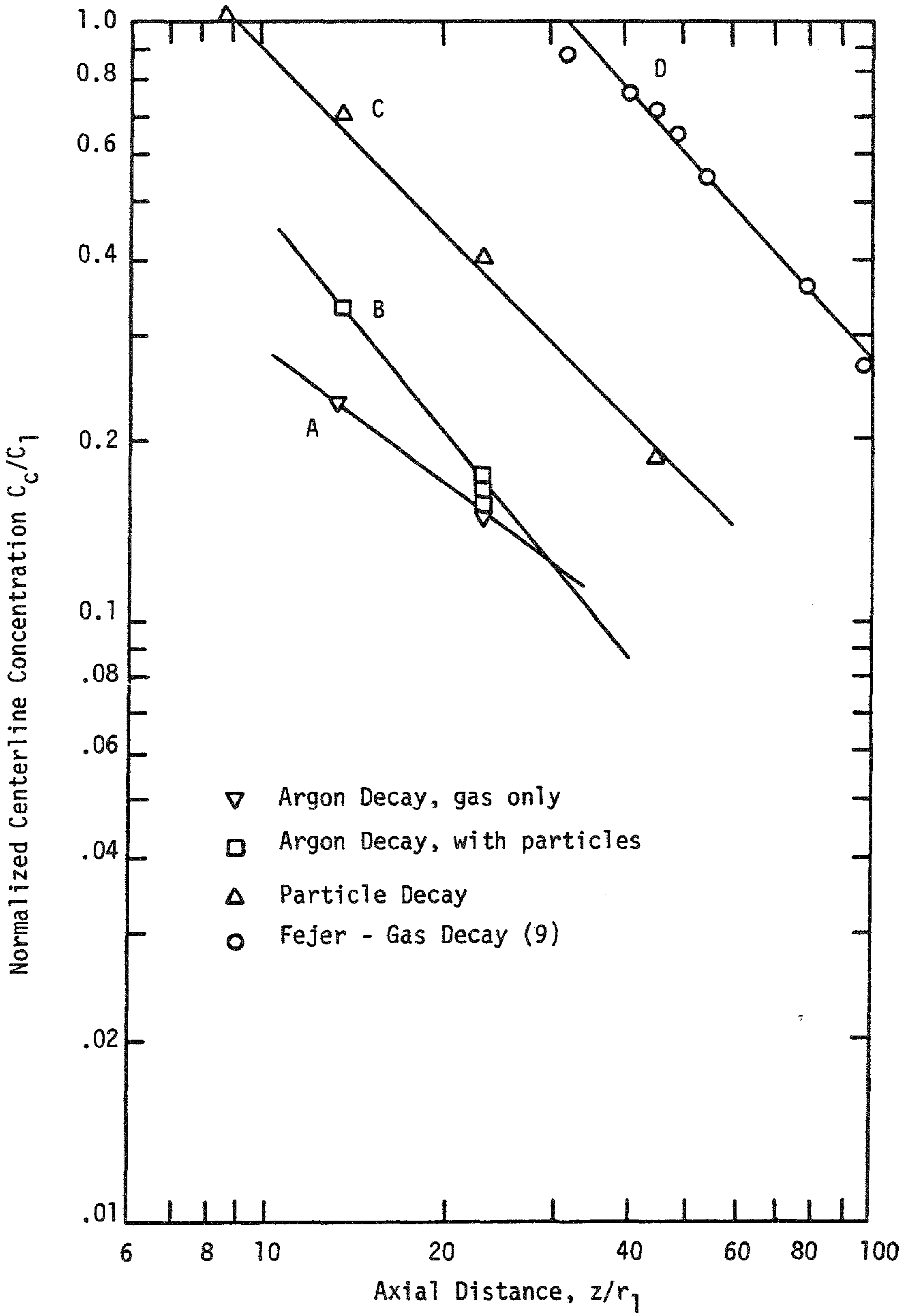

Figure 4. Centerline Decay of Argon and Silicon Particles in an Argon/Air/Silicon Confined Jet. Test Condition I (see Table 1).

will be constructed at the Research Machine Shop during this coming quarter. Installation of the components into the existing facility will occur directly after the completion of the probes. Once the system is made operable, testing with recirculation will begin. A revised test schedule with the variable parameters is shown in Table 4.

Reacting Gasification Tests

Design and Construction. In the previous progress report (10), details were presented of the final design of the high pressure coal feeder and reactor system. During the present quarter a critical path schedule shown in Figure 5 was developed for the facility construction. This critical path shows the target dates to be met in order to complete the fabrication of the high pressure gasifier by July of 1976. This will leave sufficient time for facility checkout and non-reactive tests before the end of phase 1. The critical path items are shown as the solid black bars in Figure 5. Other, less critical, but ultimately important parts of the program are shown cross-hatched. As of 31 March we were either on schedule or ahead of schedule. Specifically, the following was accomplished during the last study period:

1. All working drawings for the scrubber-feeder system, the primary/secondary injection system, and the reactor were completed, appropriate approvals have been obtained, and all materials have been ordered and received in our machine shop.

2. Fabrication of the primary/secondary parts was initiated. The design of this system was simplified somewhat from previous designs. The slight revisions resulting in the test program by this simplification are shown in Table 5.

3. After some consideration and investigation of costs, it was decided that the scrubber and feeder tanks should be fabricated by an off-campus ASTM-approved shop. Fabrication is nearly complete and delivery has been set for mid-April. After these items are received, we anticipate installation will require 2-3 weeks. The completion of the installation of the feeder will be somewhat dependent upon the availability of shop personnel to assemble the auger-gear system.

4. The secondary preheater which was ordered last quarter has now been shipped. The steam generator has been ordered with delivery indicated for May.

Two major areas which require further design work are the sampling probes and the ignition system. The probes will be used to obtain both gas and particulate samples for analysis. Experience at this laboratory has been with direct-quench, water-cooled probes, and for a first attempt, this type is being considered for this study. Initial tests of this type of probe are being planned as a part of the closely-related EPRI study using the low pressure combustor (3).

TABLE 4

REVISED TENTATIVE TEST SCHEDULE FOR NON-REACTING, RECIRCULATING FLOWS

	I		II		III		IV		V	
Parameter	Pri	Sec	Pri	Sec	Pri	Sec	Pri	Sec	Pri	Sec
Velocity, ft/sec	100	125	100	200	100	125	100	125	100	125
Pressure, psia	13		13		13		13		13	
Temperature, °F	50	50	50	50	50	50	50	50	50	200
Particle size	std.		std.		small		large		std.	
Flow rate, g/sec										
Air	5.20	542	5.20	867	5.20	542	5.20		5.20	419
Argon	16.86		16.86		16.86		16.86		16.86	
Particles	14.71		14.71		14.71		33.10		14.71	
Wt. % solids	40.0		40.0		40.0		60.0		40.0	
Mole % argon	70.0		70.0		70.0		70.0		70.0	
Sec/Pri Ratios										
Velocity	1.25		2.00		1.25		1.25		1.25	
Gas Density	0.79		0.79		0.79		0.79		0.61	
Total Density	0.47		0.47		0.47		0.31		0.36	
Gas Flow	24.6		39.3		24.6		24.6		19.0	
Total Flow	14.7		23.6		14.7		9.8		11.4	
Recirculation Diameters	I,II,III		I,II,III		I,II,III		I,II,III		I,II,III	
Axial Lengths	4		4		4		4		4	

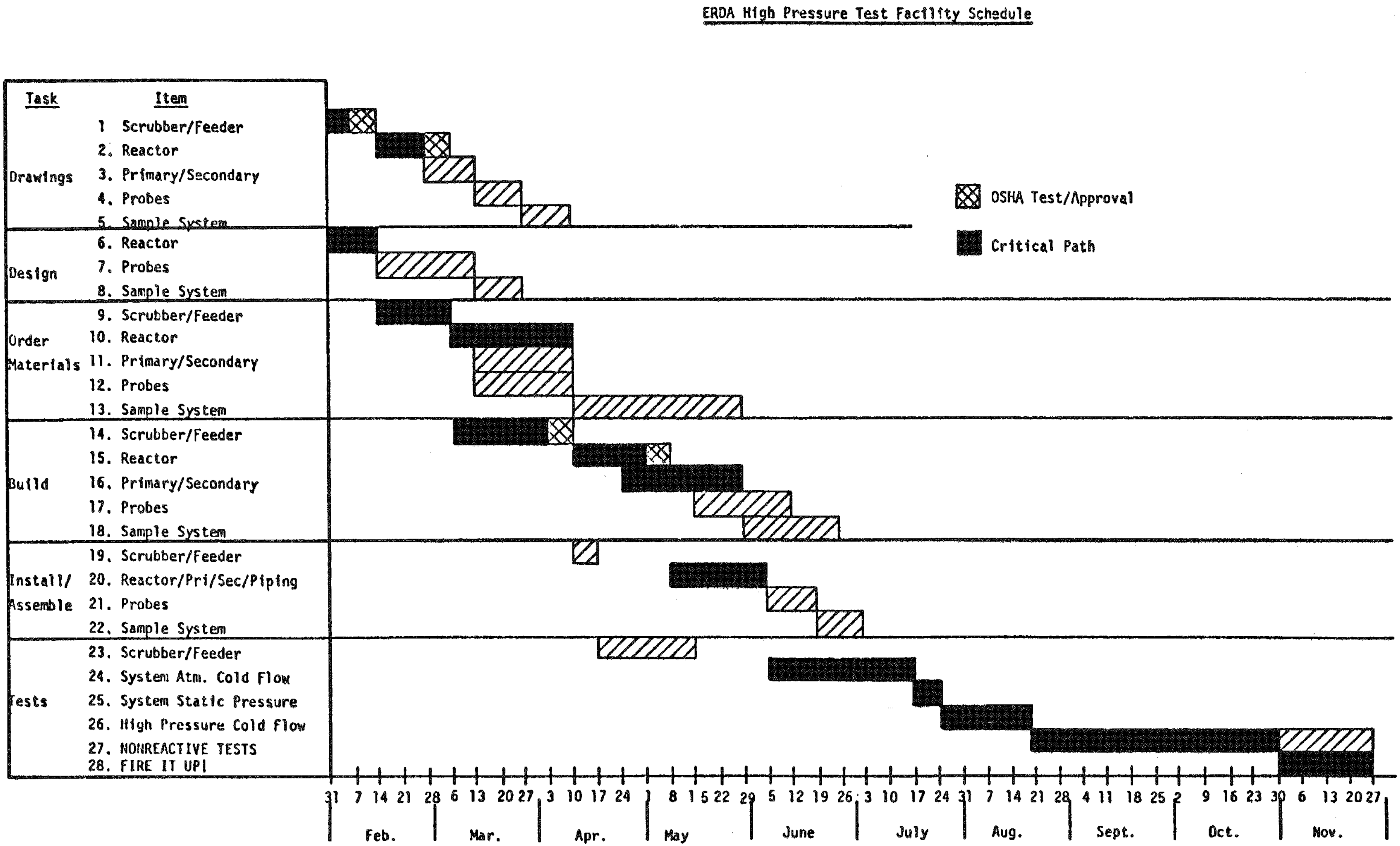

Figure 5. Critical Path Schedule for High Pressure Reactor Test Program

TABLE 5

REVISED HIGH PRESSURE GASIFICATION

TEST CONDITIONS

VARIABLE/TEST CASE	1	2	3	4	5	6	7
P, atm	10	20	10	10	1	10	10
m_c, kg/hr	136	136	136	136	68	136	68
X_c, wt %	70	70	70	70	70	85	70
Primary:							
$\dot{m}_{O_2}$, kg/hr	58.5	58.5	58.5	58.5	29.0	24.0	29.0
$\dot{m}_1$, kg/hr	194.5	194.5	194.5	194.5	97.0	160.0	97.0
U_1, m/sec	11.2	5.7	11.2	11.2	54.2	4.8	5.6
T_1, °C	82	82	82	82	82	82	82
ρ_{O_2}, g/cm^3	0.011	0.022	0.011	0.011	0.0011	0.011	0.011
ρ_1, g/cm^3	0.036	0.070	0.036	0.036	0.0037	0.070	0.036
Secondary:							
T_s, °C	316	316	427	316	316	316	316
ρ_s, g/cm^3	0.0043	0.009	0.0036	0.0043	0.0004	0.005	0.0043
U_s, m/sec	14.9	7.2	15.4	23.8	69.6	6.4	7.6
$\dot{m}_{O_2}$, kg/hr	17.7	17.7	17.7	17.7	9.1	52.2	9.1
$\dot{m}_{H_2O}$, kg/hr	52.2	52.2	52.2	52.2	26.3	52.2	26.3
$\dot{m}_s$, kg/hr	69.9	69.9	69.9	69.9	35.4	104.4	35.4
wt % H_2O	74.7	74.7	74.7	74.7	74.7	50.0	74.7
U_s/U_1	1.33	1.26	1.38	2.0	1.28	1.34	1.36

The ignition system will probably be based as much as possible on available commercial equipment. It will be necessary to preheat the interior of the reactor before the coal, oxygen and steam are introduced. Again, initial evaluation of a methane-spark ignition system is being tested as a part of the EPRI study (3).

Table 6 summarizes the current status of the major components that comprise the high pressure gasification facility.

Coal Analysis

Analysis of the quality and variability of the high volatile-B bituminous coal received from Utah Power and Light Company has continued. Six barrels of coal were randomly sampled at different levels in each barrel. The coal from different levels for a given barrel was well mixed and portions from two barrels were sent to different laboratories for ultimate analysis. The results were shown in the previous quarterly report (10). Samples were also sent to Perkin-Elmer Co. to compare the ultimate analysis obtained from an instrument they manufacture with standard ASTM techniques. A portion of their analysis has recently been received, and preliminary results from this comparison indicate good agreement on all elements.

The U.S. Geological Survey is conducting a study on the composition of western coals. Five samples have been sent to them for complete analysis, including trace metals on both the coal and ash.

The six barrels chosen for the ultimate analyses were resampled at different levels for size characterization. The samples were mechanically shaken on a Tyler 170 mesh (90 micron) screen, and each fraction was weighed and recorded. The minus 90 micron coal particles were analyzed using a Coulter Counter; the detailed results are shown in Table 7.

From the data in Table 7, the mass mean diameter and specific surface area were calculated together with statistical variation in each barrel and among barrels. These results are tabulated in Table 8. In general, the size uniformity of the coal in barrels and among barrels appears to be quite good. Barrels with wide variation can be eliminated. Initial tests will be made to evaluate the effects of these small variations in particle size on gasification rates.

During the next quarter we plan to carry out the proximate analysis on the same coal samples mentioned above, and formulate definite plans as to further treatment or classification necessary before using the coal in the test program.

Pollutant Formation

Efforts were initiated this quarter to research the question of the fate of fuel nitrogen and sulfur during gasification and what role these reactions might play in the overall process. Any compounds formed from

TABLE 6

DESIGN STATUS OF HIGH PRESSURE GASIFIER COMPONENTS

Design Item	Status	Comments
Coal/Char Feeder	In fabrication	Delivery in April
High Pressure Air Line and System	Construction and installation complete	
Particulate Removal System	In fabrication	Vessel delivery in April
Instrumentation - Recording System	Design complete	Ordered per specifications- certain components received
Primary and Secondary Control Valves	Design complete	Ordered per specifications and received
Automatic Controllers and Control System	Design complete	
Primary Heater	Design complete	Ordered and received
Primary-Secondary Injection System	In fabrication	Complete in May
Reactor Shell	Design complete - materials received	To be fabricated in machine shop - by May
Ceramic Reactor Lining	Design and testing near completion	Cylindrical cast ceramic shells
Sampling Probes	Design nearing completion	Water-cooled, direct water quench probes
Overhead Hoist System	System installed	Completed and functional
Structural Supports and System Piping	Design essentially complete	Structural supports completed
Steam Generator System	On order	Due to ship in May
Steam Superheater	On order	Has been shipped from manufacturer

TABLE 7

SIZE CHARACTERISTICS OF THE BITUMINOUS TEST COAL

Ave. Size of Increment (microns)	Barrel 2 Weight % in Increment	Barrel 2 Standard Deviation*	Barrel 8 Weight % in Increment	Barrel 8 Standard Deviation*	Barrel 13 Weight % in Increment	Barrel 13 Standard Deviation*	Barrel 18 Weight % in Increment	Barrel 18 Standard Deviation*	Barrel 21 Weight % in Increment	Barrel 21 Standard Deviation*	Barrel 27 Weight % in Increment	Barrel 27 Standard Deviation*
2.85	.41	± .05	.28	± .10	.42	± .19	.41	± .05	.30	± .06	.48	± .14
3.59	.59	.09	.37	.10	.51	.19	.50	.05	.44	.06	.51	.06
4.52	.72	.08	.47	.10	.54	.20	.60	.05	.56	.14	.70	.23
5.70	1.00	.08	.69	.20	.84	.31	.72	.14	.76	.19	.76	.18
7.18	1.60	.03	1.28	.23	1.20	.24	1.15	.33	1.21	.24	1.29	.15
9.04	2.50	.03	2.29	.41	1.99	.24	1.99	.43	2.00	.31	2.11	.23
11.39	3.65	.14	3.68	.51	3.14	.06	3.16	.62	2.97	.34	3.01	.27
14.35	4.99	.17	5.09	.54	4.28	.02	4.46	.50	4.07	.47	4.09	.19
18.10	6.48	.57	6.93	.61	6.22	.27	6.13	.66	5.52	.48	5.59	.31
22.80	8.42	.62	8.97	.64	8.48	.34	8.59	.50	7.05	.78	7.58	.27
28.70	9.82	.61	10.48	.55	10.30	.47	11.06	.18	8.95	.61	9.70	.26
36.15	10.92	.68	12.73	.43	12.26	1.21	13.28	.38	11.29	.43	11.37	.36
45.55	10.66	.74	12.16	1.05	12.24	.51	12.36	.97	11.81	.26	11.52	.77
57.40	11.47	.40	12.08	1.46	11.88	.27	12.51	.64	11.54	.79	11.70	.12
72.30	11.48	1.08	9.83	.75	9.23	.97	10.29	2.64	12.39	.58	11.85	1.07
85.30	5.66	1.30	5.34	.80	5.71	1.01	5.38	2.29	6.25	2.71	8.28	1.29
sieve cut line												
90+	9.63	1.08	7.35	1.01	10.36	.65	7.41	.45	12.89	1.82	9.46	.32

*Based on three samples taken from different levels in barrel

TABLE 8

VARIATION IN AVERAGE SIZE CHARACTERISTICS OF PULVERIZED BITUMINOUS TEST COAL

Barrel No.	Mass Mean Diameter (microns)	Standard Deviation within barrel*	Surface Area[1] (cm^2/g)	Standard Deviation within barrel*
2	39.98	±1.20	1917.22	±17.67
8	39.56	±1.48	1807.93	±111.65
13	40.14	±0.18	1819.26	±109.40
18	40.32	±1.58	1791.65	±93.99
21	42.42	±2.52	1742.08	±113.47
27	42.82	±0.83	1778.70	±70.49

*Based on three samples taken from different levels in barrel

1. Density of coal = 1.34 g/cc

Average Mean Diameter* (microns)	Standard Deviation among barrels	Average Surface Area* (cm^2/g)	Standard Deviation among barrels
40.87	±1.38	1809.47	±59.18

*Based on all six barrels

these elements may have a bearing on downstream processes by becoming catalyst poisons or atmospheric pollutants.

Sulfur is likely converted to H_2S and COS, both potential catalyst poisons. We have investigated instrumentation available to analyze for concentrations the various species of sulfur that might be found in gasifying system. We plan to initiate a review of the kinetics of sulfur reactions during gasification.

Bound nitrogen appears to be mainly converted to ammonia. However, mention is made of the fact that nitrogen dioxide may also be formed to a small extent (11). We intend to expand our literature base and define our research goals in this area during the next quarter.

Coal Gasifier Model Development

Model Basis. During the previous study period, the basis for a computerized model for predicting characteristics of entrained coal gasifiers was developed. The model uses the integrated or macroscopic form of the general conservation equations for a volume element inside the gasifier. The following aspects of pulverized coal gasification have been included in the model: (1) mixing of primary and secondary streams; (2) recirculation of reacted products; (3) pyrolysis and swelling of coal; (4) oxidation of the char by oxygen, steam and carbon dioxide; (5) heat transfer between the coal/char particles and gases; (6) variation in composition of inlet gases and solids; (7) variation in coal/char particle size; (8) oxidation of the hydrocarbons produced from coal pyrolysis. A summary of key model assumptions and conditions was given in Ref. 10.

Differential mass, energy and momentum balances were developed for particle and gas phases and were summarized in Ref. 10. This set of first-order, non-linear equations required also a large number of auxiliary, algebraic equations as component model parts. These equations describe the following aspects of the coal gasifier process: (1) enthalpy-temperature relationships; (2) physical properties including heat capacity, thermal conductivity, diffusivity, and viscosity; (3) radiative interchange inside the gasifier; (4) equations of state and mass flow continuity; (5) convective and conductive heat interchange among the gases, particles and walls; (6) rates of pyrolysis and oxidation of coal and char; (7) rates of oxidation of gaseous hydrocarbon products. A summary of these equations was also given in Ref. 10.

Model Solution. During this past quarter, model equations were checked in detail for consistency and accuracy. Then, a general scheme for computer-solution of the equations was developed, as shown in Figure 6. This solution scheme incorporates an existing generalized thermochemical program for calculating equilibria in complex gases (12). The solution technique requires an initial assumption for the axial temperature profile along the gasifier. From this assumption, radiative heat transfer within the gasifier can be computed, and then the set of differential equations integrated along the gasifier. Included in this integration is the revised temperature profile which is used in the next iteration. This process is repeated until the solution converges.

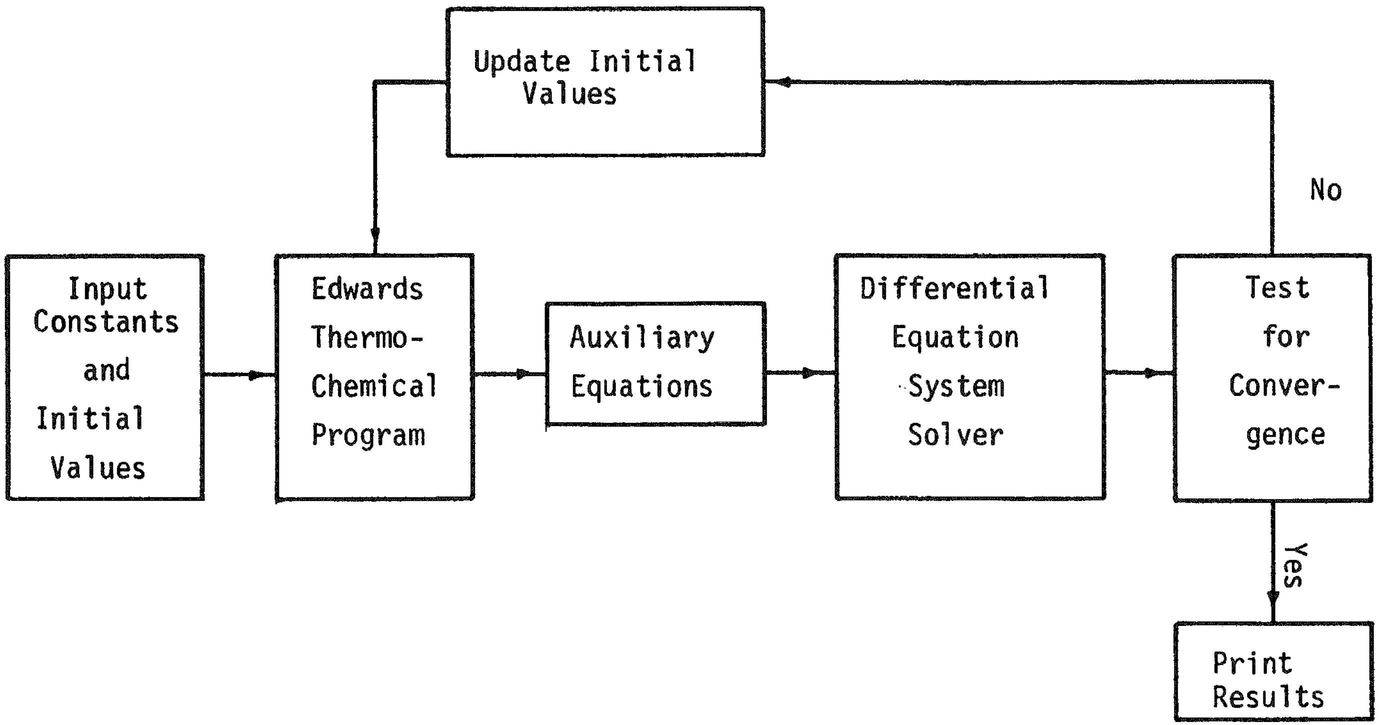

Figure 6. Information Flow for Differential Equation Solution

Programming of this solution technique is nearly completed. First debug runs will be attempted during the next study period.

Other Activities

During this report period, the follow-on proposal for phase 2 of this study was completed and mailed to ERDA. This proposal included a proposed program addition for development of gasifier predictive techniques.

Plans for presentation of a paper based, in part on this work, at the American Chemical Society Meeting in New Orleans in March of 1977 were made. When the preliminary draft is prepared, it will be submitted to ERDA for publication approval.

A paper summarizing work on this study was presented at the First Rocky Mountain Fuels Symposium, held at Brigham Young University in late January.

PLANS FOR THE NEXT STUDY PERIOD

During the sixth quarter of this investigation, the following plans have been identified:

1. Continue technical review and analysis of coal literature, emphasizing coal pyrolysis, volatiles combustion, recirculating flows, and related topics.

2. Continue conducting tests and analyzing test data for non-reacting, non-recirculating, particle-laden flows.

3. Complete fabrication of all major components for the laboratory scale coal gasifier and initiate assembly and check-out in the combustion laboratory.

4. Complete computer programming and debugging of the macroscopic coal gasification model and initiate trial computer solutions.

5. Complete fabrication of the probe section for the non-reacting, recirculating test facility.