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MIXING AND GASIFICATION OF COAL
IN ENTRAINED FLOW SYSTEMS

Quarterly Technical Progress Report No. 5
for the Period 1 April 1978 to 30 June 1978

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FOREWORD

This report summarizes technical progress accomplished during the fifth report period of a two-year study being conducted for the Department of Energy (DOE) under contract No. EF-77-S-01-2666. This work period was 1 April 1978 to 30 June 1978. Work was accomplished under the direction of Dr. L. Douglas Smoot, principal investigator, Dr. Richard W. Hanks, and Dr. Paul O. Hedman senior investigators. Dr. Robert C. Wellek is the Program Manager for DOE.

Graduate and undergraduate students who have contributed to the technical progress and to this document were John Baardson, Rick Guercio, Stanley Harding, Don Leavitt, Lyle Richins, Jerry Sharp, Douglas Skinner, and Philip Smith. Mr. James Hoen, Supervisor of the Research Machine Shop, has provided assistance in design and construction of reactor components. Michael King, Elaine Alger, and David Creer have provided technician, typing and drafting services. Subcontract work at the University of Utah on generalized model development is being conducted under the direction of Dr. David Pratt with Dr. John Wormeck and Miss Angela Varma.

ABSTRACT

This report summarizes work completed during the fifth quarter of a two-year study to investigate mixing and gasification of coal in entrained flow systems. This is the second phase of a study that was initiated in November, 1974.

During this report period, 26 atmospheric, cold-flow mixing tests were completed with 21 yielding final data. Flow asymmetry problems were encountered when using nonparallel injection into the recirculation chamber. Attempts to align the test system improved but did not completely resolve this problem. Revised methods of data analysis further improved interpretation of these data. Most previous cold-flow tests were conducted with a very short test section following the probe collar and then a sudden reduction in flow area. New tests with longer aft-test sections showed little effect of post test section length on measured mixing profiles.

The gasifier has been modified and several parts of the system pressure-tested in anticipation of starting the high-pressure cold-flow test program. A new back-pressure regulator has been ordered.

Eleven atmospheric gasification tests were performed with the gasifier during this period. The prototype sample probe has been shown to work and the complete probe-sample collection system has been designed and constructed. An over-pressurization of part of the gasifier exhaust system resulted in a failure and month-long interruption of testing occurred while a new system was installed. Testing has now been resumed.

Predictions were made with the one-dimensional coal gasifier computer model for the 5 ST/hr Bi-Gas gasifier, and the Coates entrained gasifier and results were compared with limited measurements.

Work has continued on the generalized two-dimensional gasifier model. The probability distribution function formulation to describe diffusion-limited gas-phase combustion has been completed and tested. Thus, the two-dimensional code is now functional for gaseous systems.

OBJECTIVE AND SCOPE OF WORK

Background

The recent emphasis on the energy requirements of our country and the necessity of importing a large fraction of our petroleum fuels has clearly demonstrated the need to develop alternate energy sources. The majority of available domestic energy resources cannot presently be used directly without degrading the environment beyond that specified by current environmental laws. It is becoming increasingly apparent that the development of adequate energy supplies and the maintenance of an adequate environment ranks high on the list of national priorities and will represent prime determining factors in the setting of domestic and foreign policies for years to come (1). It is possible that nuclear, geothermal, or solar energy may eventually meet part of this increasing energy need. However, with our present level of technology, we may not be able to supply all of the increasing demands economically from these sources during the present century. As a consequence, we are required to convert energy from fossil fuels into a more desirable form as an intermediate solution to the energy problem (2,3).

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 at all well understood and appear to require considerable study before optimum engineering designs are possible. One such problem associated with the entrainment of the coal particles is the influence of the turbulent mixing characteristics of a particle-laden gas stream on chemical reactions which take place in the reactor, and on the subsequent yield of products. Questions such as, "How can the reaction vessel best be designed to maximize yields of desirable products" cannot be answered until the details of these processes are understood. Such mixing problems have been identified (4) as among the most critical and key problems which need to be solved in order to render the design of entrained gas reactors practicable. It is therefore important to conduct a detailed and intensive study of the turbulent mixing of particle-laden gas streams and the chemical kinetics and reaction yields of entrained coal particle reactors.

While some work has been and is being conducted (5,6) 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, a continuation of the recently completed Phase 1 ERDA study on coal mixing and gasification in entrained systems (7), 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. The effect of reactor geometry is being given particular emphasis in a series of entrained-flow, laboratory-scale experiments. Potential design models for coal gasifiers and combustors are being developed and evaluated. Specific tasks that have been outlined for accomplishment during the Phase 2 study are listed below.

1. Cold Flow Tests. Complete the non-reactive, atmospheric and high pressure cold flow tests initiated under Phase 1. Atmospheric tests will emphasize recirculation effects in ducts of several different diameters. The purpose of the high pressure tests is to determine the effects of pressure as an operating variable on gas and particle dispersion rates for various operating conditions, stream composition, and inlet jet geometric configurations.

2. Reactive Flow Tests and Analysis. Conduct a series of gasification experiments using char and coal particles. Measure locally in the reacting system the extent of particle dispersion, the extent of gas mixing, the amount of particle reaction, the local product composition, the extent of pollutant formation, and the temperature and/or velocity distributions.

3. One-Dimensional Coal Gasifier Model Development and Application. Complete the development of the macroscopic computerized mathematical model for describing the reacting coal gasification or char combustion processes. Include recirculation effects and also include available theory and measurements on the behavior of char or coal particle reaction and on gas/particle dispersion. Investigate the characteristics of the model and conduct parametric studies to determine relative tradeoffs resulting from variation in controllable parameters. Compare model predictions with measured results and deduce dominant processes that occur during these particle reaction sequences.

4. Generalized Gasifier Model Development. Continue the development of a generalized, multi-dimensional model for describing entrained coal gasification processes. This task has four parts as indicated below.

a. Component Development. Continue the technical development and improvement of the various model components being used in the generalized entrained coal gasification code. Emphasis is being given to particle flow, radiation, and coal reaction aspects.

b. Model Parameters. Determine suitable model parameters for inclusion in the model code. These include 1) turbulence coefficients, 2) chemical rate coefficients for gas phase reactions, 3) turbulence coefficients for random particle motion due to gas turbulence, 4) coal reaction parameters for pyrolysis and heterogeneous oxidation, and 5) radiation parameters for interchange among coal/char particles, gas and walls.

c. Model Efficiency. Investigate methods to reduce the required computer storage and/or solution time in order to improve the model performance and efficiency.

d. Model Computations. Perform model computations for pulverized coal gasification and combustion at the test conditions of the DOE/EPRI studies. Compare the model predictions to the experimental results.

Technical Approach

In order to accomplish the tasks outlined above, an entrained flow gasifier has been designed and constructed. The gasifier has been designed to operate at a peak pressure of 2000 kPa (20 atm). The high pressure gasifier has been developed principally to study entrained coal gasification processes at elevated pressures, and has been constructed using funds from this study. The gasifier has a primary nozzle diameter of 12.7 mm, and a coal processing capacity of 13.6-136 kg of coal per hour. A series of non-reacting, high-pressure tests using this reactive high pressure test facility is also outlined as a part of this study during Phase 2.

A second test facility is also available at this laboratory and is being used for this project to study mixing in cold flow, particle-laden streams at atmospheric pressure conditions. Experimental results for Phase I included a series of non-reacting, atmospheric tests using this existing atmospheric, non-reactive test facility (7).

The basic experimental approach used in the reactive tests is to obtain a particle/gas sample from the reactor using specially designed probes. Water-quenched probes are used to provide water directly to the gas-particle mixture in order to rapidly terminate chemical reaction and to keep ash/slag from adhering to probe walls. Separate key chemical components are placed in the primary and secondary flows. Analysis of the key tracers from primary and secondary streams indicate directly the extent of gas-phase mixing at the point the sample is collected. Further, particulate materials in the sample are separated and analyzed to determine the rate of particle dispersion and also to determine the ash, volatile matter, and possibly sulfur and nitrogen content for the reacting cases. Reacting gas samples will also be analyzed to determine such quantities as CH_4, CO, CO_2 and H_2. This information provides direct measurement of the extent of gas-phase mixing, the extent of particle-gas mixing, the extent of coal or char gasification, and possibly the extent of sulfur and nitrogen pollutant formation. Such detailed information on local chemical composition serves as the basis for interpreting rates of mixing and particle reaction, and therefore influences of mixing rate on particle reaction rates.

This general approach was successfully used in analyzing boron particle mixing and combustion effects in a high pressure reactor (8) and has also been applied by this laboratory to coal/air combustion (6).

During Phase 1, a one-dimensional model of entrained coal gasification was developed (7). This model includes effects of recirculation, radiation, particle-gas mixing, coal pyrolysis, char oxidation, and gas-phase reaction. Basic macroscopic equations of change (9) were used. Since the model has a general one-dimensional nature, recirculation and particle-gas mixing rates of primary and secondary streams are required input into the model. Also during Phase 1, a computer solution of this model was nearly completed, and some of the characteristics of the model were investigated.

During Phase 2 the model is being studied in more detail. A series of parametric runs, investigating both required physical and chemical parameters and controllable gasifier conditions and geometries is being made. Model results are being compared, where appropriate, with coal gasifier measurements. The model will also be applied to the analysis of data from Coates' (10) high-pyrolysis-rate-gasifier project which is being funded by DOE.

Comparison of model results with test results of Task 2 above is limited. The model does not predict radial variation of properties inside the gasifier. Experimental data do provide both axial and radial distributions of these properties. Even so, the model results should be very useful in interpreting test data, in exploring general characteristics of coal gasifiers, and in guiding the development of more complex models.

During an independent study sponsored by EPRI (11), work was initiated to develop a generalized, multi-dimensional model of coal gasification processes which will remove many of the restrictions inherent in the one-dimensional model. During Phase 2, development of this generalized model will be continued under DOE sponsorship.

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. Cold Flow Tests.

Twenty-six atmospheric pressure cold-flow mixing tests were performed during the reporting period of which twenty-one yielded final test data. A set of tests were made with nonparallel injection into the largest duct (343 mm diameter). Flow asymmetry problems were observed and steps are being taken to correct the difficulty. A second set of tests was performed with parallel injection into the medium size (260 mm diameter) duct but with ducts of different overall length. The objective of this set of tests was to determine the effect of the length of mixing duct which extended beyond the instrument collar. The data show that the overall duct length has little effect on the observed mixing rates of gas and particles.

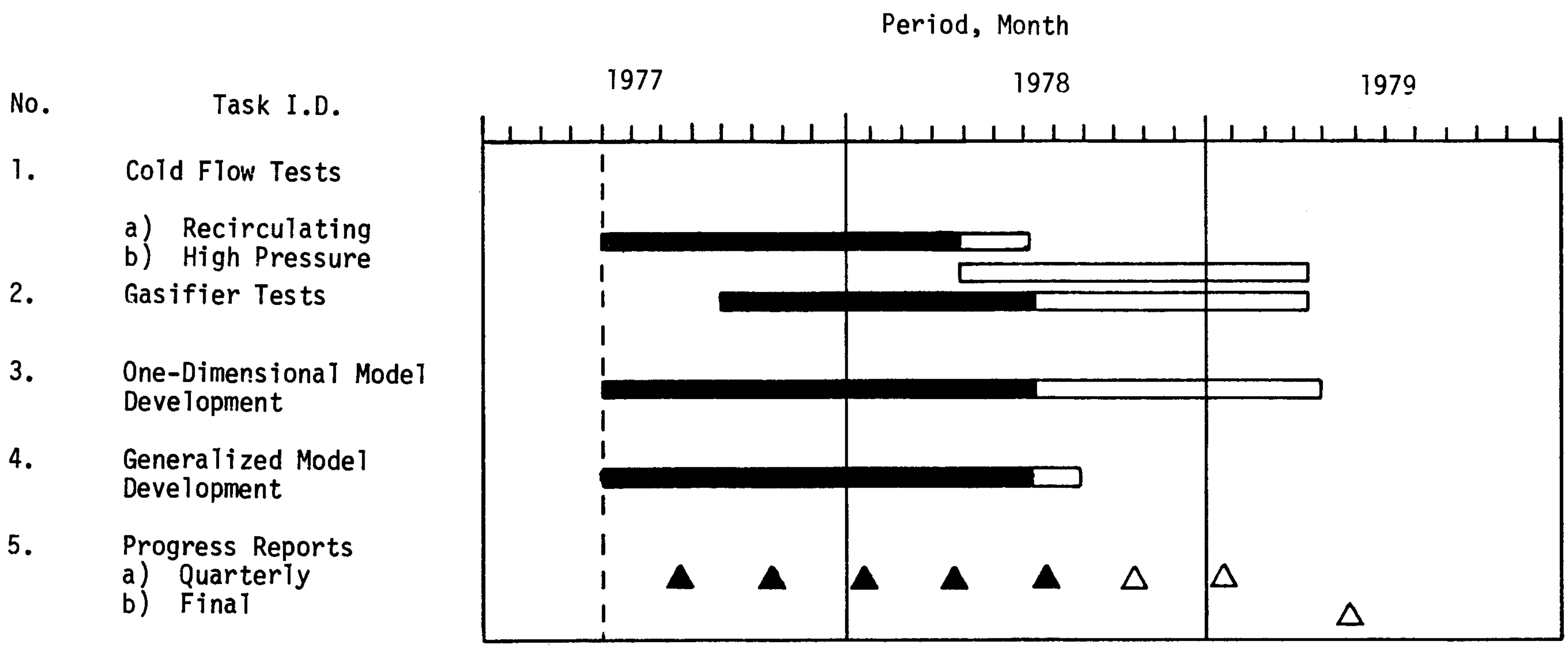


Figure 1. Summary Chart of Phase 2 Research Activities.

Several modifications have been made to the gasifier and the existing air supply system in preparation for high-pressure, cold flow coal-air mixing tests. Pipe fittings, pressure gauges, and tranducers suitable for the range of pressures to be studied have been installed and made operational. Also, the surge tanks and associated piping have been pressure-tested to 800 psi.

Task 2. Gasifier Tests and Analysis.

An additional eleven reactive tests were made with the gasifier this quarter to check out the facility, and the prototype probe and sampling system. To date a total of 26 reactive tests have been conducted. An overpressure in the exhaust gas system occurred on test number 25 which separated several hose clamp joints in the exhaust system. Replacement of this exhaust system with a welded-steel system delayed testing for about one month. The repair has been completed and testing has resumed.

The prototype probe and sample system have been used successfully on six tests. The final design of the probe and sample collection system has been completed and fabrication initiated. It is expected that the first tests with the complete bank of probes will begin early next quarter.

Task 3. One-Dimensional Coal Gasifier Model Development.

The one-dimensional gasification/combustion model was applied to several additional reactors including the BYU Rate Resolution Combustor, a 5 ST/hr Bi-Gas gasifier, and the Coates entrained gasifier. The later two are both under development by DOE. The application of the one-dimensional code to different reactors has lead to code modifications which have improved model efficiency and performance. Parametric studies are being continued to evaluate the effect of gasifier operating variables on gasifier performance.

Task 4. Generalized Gasifier Model Development.

Work on the multi-dimensional model has continued. The probability distribution function (PDF) formulation to describe diffusion-limited gas-phase combustion has been completed and tested. The code is now functional for gas-phase systems.

Task 5. Progress Reports.

This report represents the fifth quarterly report on the current DOE contract. Plans were also made to attend the annual DOE University Contractor's meeting in Lexington, Kentucky.

DETAILED DESCRIPTION OF TECHNICAL PROGRESS

Technical Visits

Visits were made by L. Douglas Smoot to Foster-Wheeler (Livingston, N.J.) and Babcock and Wilcox (Alliance, Ohio) where technical discussions on coal, gasification, and combustion were held. Additionally L. Douglas Smoot participated by invitation in a coal conference hosted by EPA in Los Angeles, Ca. Also, during the quarter, Paul Hedman participated by invitation in an EPRI coal gasification modeling conference in Pacific Grove, California, and in a Combustion Diagnostics Short Course at Purdue University.

Atmospheric Cold-Flow Tests With Recirculation

During this report period, 26 cold-flow mixing tests were performed, of which 21 provided final data. At the beginning of the quarter, tests were performed under flow conditions I and II (12) (the standard flow condition both without and with particles) and using the nonparallel (30°) secondary injection with the large (343 mm diameter) mixing chamber.

Asymmetry of the mixing streams was observed in the first test and the first three tests performed were attempts at correcting this asymmetry problem. It has been found that the primary tube was improperly inserted into the system causing some leakage of the primary stream into the secondary stream before the mixing section.

Table 1 is a summary of the data collected for these nonparallel large recirculative duct tests and Figure 2 is the axial decay plot for these tests. An attempt to correct the data to account for the asymmetry observed has been made by referencing the data to the flow center as opposed to the geometric center. The corrected test data appear to be much more consistent, as indicated by the accuracy of fit of the radial decay profiles and the agreement between the calibrated and integrated particle mass balance in Table 1. Also, the axial decay plot shows the particle data to be very linear on the log-log plot. The displacement of the flow center with respect to the geometric center also gives a measure of the degree of asymetry in the duct. It is planned to reproduce these tests once the hardware problem has been corrected.

Figure 2 shows the axial decay plot for these tests in comparison with other tests performed by Memmott (13) and Tice (14) for Flow Conditions I and II. Memmott's tests were performed using nonparallel secondary injection without the expanded mixing chamber, and Tice's tests were performed using parallel secondary injection with the expanded mixing chamber. Comparison of the particle data for these tests (first three lines on the right side) shows that use of the nonparallel injection with recirculation enhances the rate of particle mixing. Comparison of the gas data shows that for flow condition I, the rates of gas mixing for the three flow geometries are essentially the same (having

Table 1

SUMMARY OF COLD FLOW TESTS USING NONPARALLEL SECONDARY INJECTION WITH THE LARGE SIZE MIXING CHAMBER

TEST NO.	FLOW COND	AXIAL PROBE LOCATION (m)	ASYMMETRY CENTER[3] (m) ARGON	PARTICLE	RADIAL PROFILE ACCURACY OF FIT[4] ARGON	PARTICLE	PARTICLE MASS BALANCE[5]
29	I[1]	0.152	0.047	-	0.986	-	-
25	I	0.305	0.033	-	0.984	-	-
27	I	0.457	0.031	-	0.975	-	-
28	II[2]	0.152	0.048	0.014	0.989	0.999	-2.5
24	II	0.305	0.028	0.037	0.979	0.999	12.0
26	II	0.457	0.017	0.045	0.987	0.995	6.4

[1]Standard flow condition without powder.

[2]Standard flow condition, with powder.

[3]Distance from calculated asymmetric centerline to geometric center of duct.

[4]Index of correlation, r^2, from statistical curve fit.

[5]Percent error between calibrated mass flow and integrated mass flow from the data.

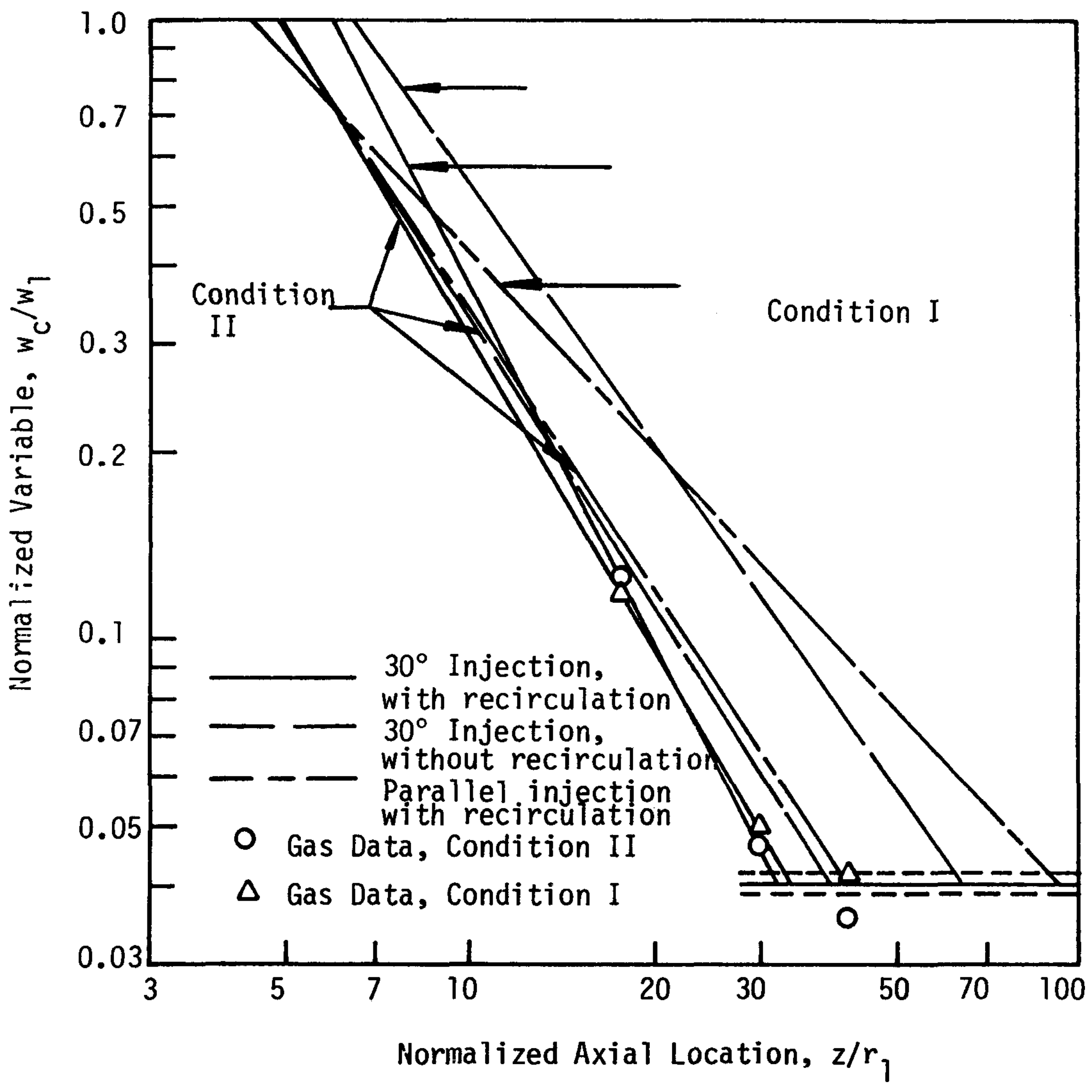


Figure 2a. Gas Axial Decay Data for Flow Conditions I and II, Using Both Parallel and Nonparallel Secondary Injection With and Without Expanded Mixing Chambers.

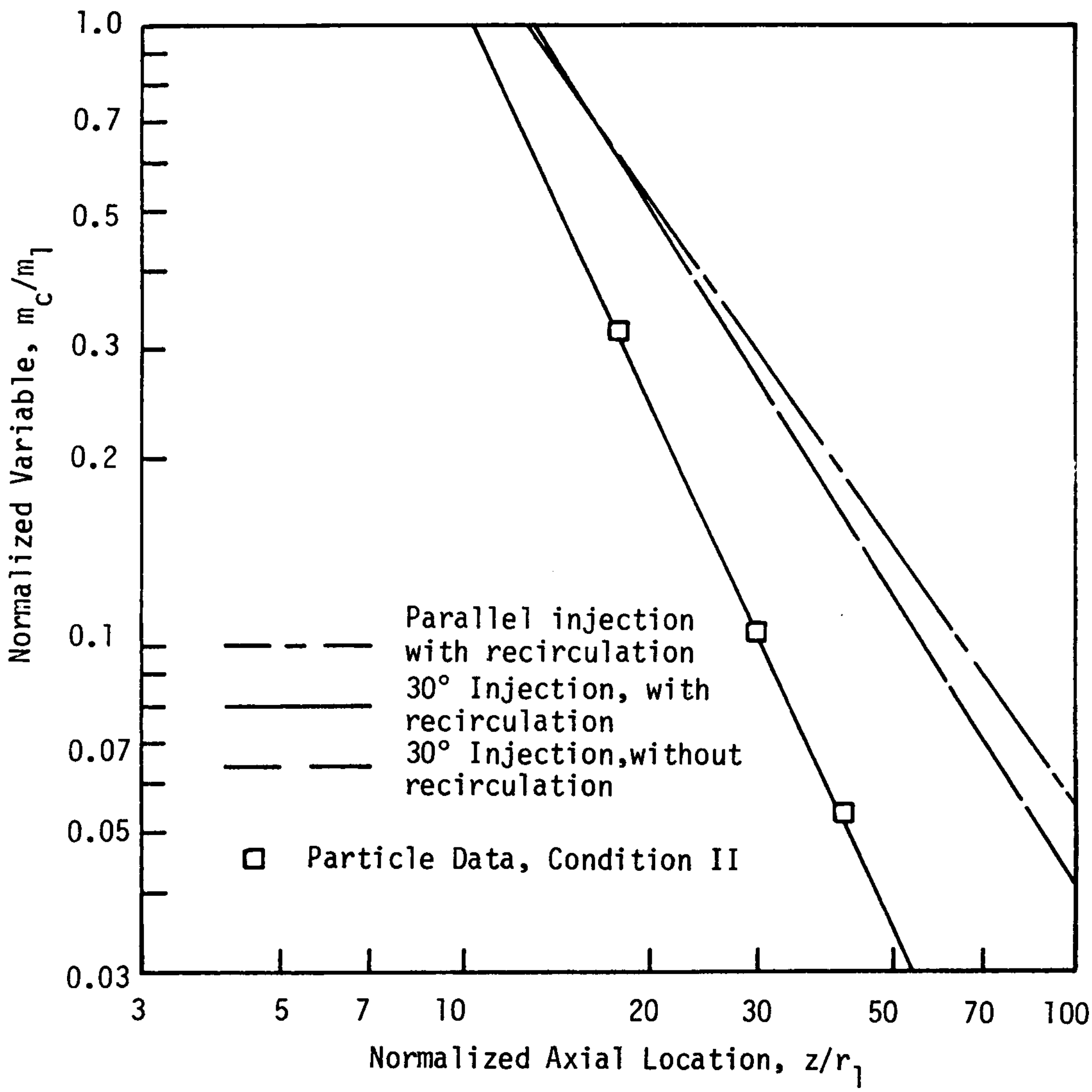


Figure 2b. Particle Axial Decay Data for Flow Condition II, Using Both Parallel and Nonparallel Secondary Injection With and Without Expanded Mixing Chambers.

a normalized core length, z/r_1, of about 4.8). For flow condition II, the data indicate that the nonparallel injection without recirculation gives the best rate of gas mixing. It is not known to what extent the leakage of the primary stream into the secondary stream has influenced the data and therefore, these results are only preliminary.

At the end of the quarter, seven additional tests were performed using the same flow conditions and flow geometry described above. These tests were performed to confirm the results and data just discussed. In these tests, as in the tests previously performed, asymmetry of the mixing streams was again observed, even though the hardware problem had been corrected and the primary duct had been mechanically aligned with the mixing chamber. It is now thought that this asymmetry is being caused by nonuniform flow of the secondary stream through the nonparallel injection collar. The data reduction for these tests is now being performed and the results will be reported in the next report.

The other tests performed during this report period correspond to flow condition II (standard condition with standard powder) using the parallel secondary injection with the medium (260 mm diameter) mixing chamber. The purpose of these tests was to determine the effects on mixing of the overall mixing-chamber length. In recirculation tests performed previously on the cold-flow test facility (14), the overall mixing-chamber length was varied with the axial position of the collection probes, with the collection probe collar always being the last section of the mixing chamber. In the current tests the overall length of the mixing chamber was fixed at two different lengths (610 mm and 914 mm) and did not vary with the axial location of the probe collar. For comparison purposes, two tests were performed using a variable length mixing chamber (305 mm and 457 mm). The results of these constant chamber-length tests are shown by the axial decay plot of Figure 3. Comparison of the data points and the axial decay lines indicate that changing the duct length has little effect on the gas mixing data. Although some variation in the rates of mixing of particle data is observed, it is thought that the rates observed are within the accuracy of the data and that the effect is small. Therefore, it is concluded that the length of the mixing chamber has very little effect on the particle and gas mixing rates.

Also during this report period, it was found that particle erosion had damaged a few of the small-diameter, isokinetic pressure taps in the sample probes. These eroded tubes have been replaced and testing has continued.

Plans for the next quarter call for continuation of testing according to the test schedule outlined in Table 2.

High Pressure Cold-Flow Mixing Tests

Several modifications were made to the existing air supply facility to handle high pressures for the high-pressure, cold-flow coal air tests. Pipe fittings and pressure gauges were installed

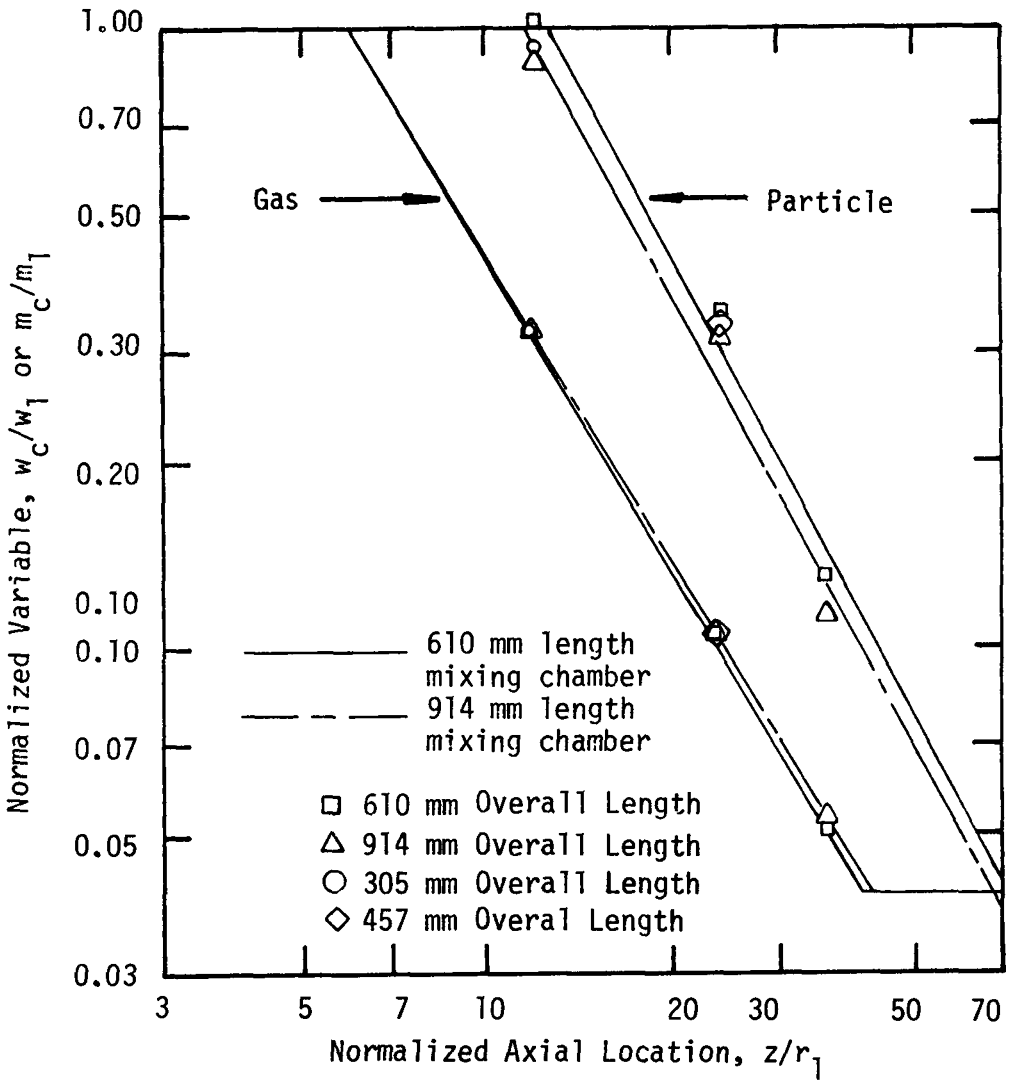


Figure 3. Effects of Mixing Chamber Length, Flow Condition II, Medium Recirculation Chamber, on Mixing Rate.

Table 2

Test Schedule for Cold-Flow Facility Test Series 3

FLOW CONDITION	I	II	III	IV	V
FLOW CONFIGURATION (RECIRCULATION DIAM. AND INJECTION ANGLE)	(REFERENCE GAS ONLY)	(REFERENCE)	(SMALL SILICON)	(COAL)	(HIGH VELOCITY SECONDARY)
Small Diameter Parallel	---	5	4	(3-4)	---
Small Diameter 30°	(3-4)	(3-4)	---	(3-4)	(3-4)
Med. Diameter Parallel	4	6	---	---	---
Med. Diameter Parallel Constant Length Mixing Chamber	---	6	---	---	---
Med. Diameter 30°	---	---	---	---	---
Large Diameter Parallel	---	---	---	(3-4)	---
Large Diameter 30°	6	6	---	(3-4)	(3-4)

Note: Numbers in parenthesis indicate estimated number of tests which will be run. Numbers without parenthesis indicate tests completed. Total tests planned - 57-65 tests.

that are suitable for the desired pressure range Transducers, thermocouples, switches and wiring were designed and installed in the existing air flow control apparatus to have accurate control over high pressure and air flow. Since installation, the air control facility, along with surge tanks and copper lines, have been tested to 800 psi.

Also, a back-pressure regulator has been ordered to control the high pressure in the coal gasifier for non-reacting tests as well as reacting tests. The sampling system has been designed and partially built. Pending arrival of the back-pressure regulator, it is anticipated that the cold-flow high-pressure testing sequence will be initiated in the next quarter.

Gasification Tests

Test Facility. During this quarter, eleven additional experimental runs were made in an attempt to check out the test facility, prototype probe and sample collection system. To date, 26 tests have been conducted. Table 3 presents a summary of the recent tests, together with their objectives and results.

A delay in testing of nearly a month was incurred as the result of an overpressure in the combustion laboratory exhaust system which occurred while attempting to ignite a natural gas-oxygen mixture at atmospheric pressure in order to preheat the reactor in run 25. Several hose clamp type joints in the gas discharge piping which leads from the scrubber to the building roof were separated. The cast iron pipe with hose-clamp joints has been replaced with a schedule 40 steel pipe with welded joints. Also, burst disks will be placed in the gas discharge piping both upstream and downstream from the back pressure regulator. One major contributing factor leading to this incident was that the prototype probe, housed in the same section as the sight glass, had been moved to the bottom of the gasifier, and visual confirmation of ignition was thus made more difficult. A second sight glass had been planned but had not been installed at the time of the incident. This situation has since been remedied. In addition, the written start-up procedure has been revised to include a purge of the reactor vessel if natural gas-oxygen ignition is not obtained promptly, in order to remove unburned, potentially explosive mixtures from the gasifier and exhaust piping.

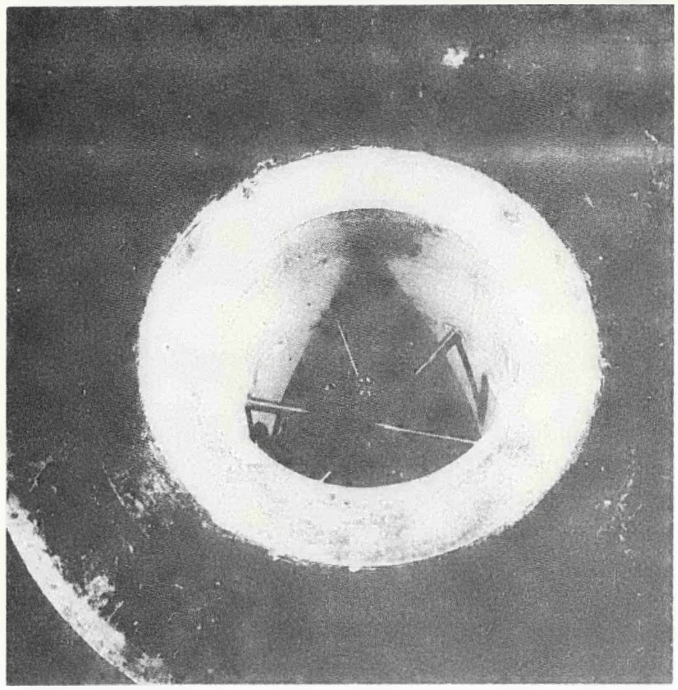
During the interruption of testing the gasifier probe section was lined with castable ceramic and readied for multiple-probe runs. Figure 4 shows the probe section with the sampling probes in place. It is anticipated that multiple-probe runs will begin shortly after the fabrication of the sample collection vessels is completed.

The regulator, which had previously been purchased for use as the back-pressure controller, was found to be unsuited for this application and a replacement has been ordered with delivery expected in the first week or two of the next quarter. Check-out of the facility at elevated pressure will begin after this regulator has been installed.

Table 3

Summary of Gasifier Test Results

Test No.	Objective	Results
16	Test probe/sampling system check out scrubber cyclone	Pressure drop through cyclone too high for atm.-pressure runs-ran on bypass - blew 2 primary burst disks no sample
17	Test probe/sampling system; 0.238 cm orifice in sampler	Collected ~0.5 gm solid sample durin coal/O_2 flame - added steam success-fully - no gas sample obtained
18	Test probe/sampling system; 0.238 cm orifice in sampler; centerline, down 24 cm	Successfully established coal/O_2/ste flame - probe water flashed - probe slagged over - found pri tube fallen fiberflax liner eroded - replaced bo and cleaned probe
19	Test isokinetic probe/ sampling system - 0.159 cm orifice in sampler; center-line, down 21.6 cm	Checked for isokinetic sampling duri heatup with CH_4/O_2 flame ~8 ml/sec water flow gave isokinetic sampling collected ~0.64gm solids, no gas - some scrubber problems leading to flame instability - need to clean scrubber more often
20	Repeat test 19 except ran longer to get gas sample	Scrubber problems - char plug in dis charge - sampled ~0.45 gm solids, no gas
21	Repeat test 19 except removed sample orifice	Successful coal/O_2/steam flame - obtained ~1.67gm solids and gas samp
22-23	Confirm high collection rate from Run 21	Sampling system plugged - need to provide capability of blowing probe/ sampling system clear of obstructior before sampling
24	Same as runs 22-23	N_2 purge enabled run to progress aft incipient plugging noticed - obtaine 1.7gm solid - successfully sampled t gas
25	Test probe/sampling system at 102 cm down	Need to syphon to establish water fl to sampler - ignition difficulties c to low sight window position - over-pressure blew out gas exhaust pipin
26	Test probe/sampling system at 102 cm; two sight windows, sample collection vessel horizontal	Had problems with sample water on ignition - possible plug in probe



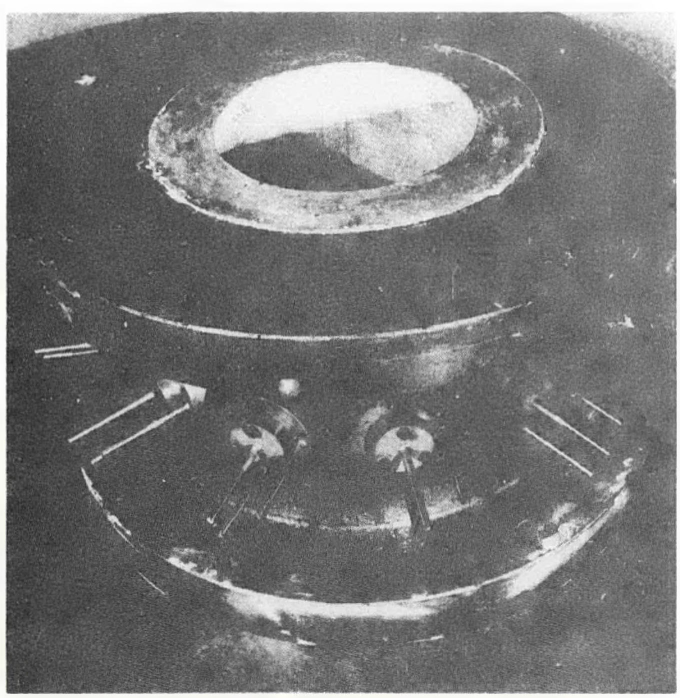


Figure 4. Photographs of Finished Probe Section with Battery of Probes in Place.

Coal Analysis. In a previous report (19), the use of atomic absorption spectroscopy to determine the amount of iron in coal samples was shown to lead to erroneous results because the particulate matter in the samples could not be completely dissolved. As an alternative to this, x-ray fluorescence measurements were made on samples from the combustor and samples of coal ash. From these results, it was also shown that the amount of iron varied but that aluminum remained more nearly constant. Therefore, approximately 30 char samples from various combustion tests were analyzed using this method. The percent of coal burned as calculated by Al_2O_3 is plotted versus the percent burnout calculated by the ash. The results are shown in Figure 5. In order to calculate the amount of coal burned using aluminum, a coal sample of known ash content had to be analyzed so that 0% burnout compositions could be obtained. This was done for a coal sample with high ash content (9.5%) and for a sample with low ash content (7.2%). If the burnout predictions were identical using the two methods, the results would fall upon the diagonal line.

From the previous work on ash solubility and volatility, it was postulated that using ash as a method of predicting burnout would give somewhat lower results. And, the greater the ash in the sample the worse the prediction would be. For Figure 5, the computations based on 9.5% ash in coal gave somewhat higher results up to about 75% burnout, and then gave identical results. This is just opposite to what was expected. Perhaps the supposed effects due to ash volatility and solubility just countered each other and no loss of ash was obtained. From the graph, the 7.5% ash in coal samples gave consistently lower results; however, they do approach the diagonal again at higher burnouts.

In essence, Figure 5 gives a range of possible values for the burnout calculated by aluminum. Since a sample of raw coal from each run was not obtained, a definite correlation cannot be made. Therefore, the major conclusion and recommendation is the need for accurate samples of both the raw coal for each run and ample samples from the probes.

Sample Train. The single probe sample system has been functioning quite well during this report period. A slight modification of the probe tip seems to have overcome some plugging problems. Approximately six samples have been collected and analyzed. A typical result is shown in Table 4.

Also, during this quarter a complete set of seven probes was fabricated (see Figure 4). The final design of the entire sample collection system was finished and the fabrication is expected to be completed early next month. A schematic diagram of the system is shown in Figure 6. The entire system is made of stainless steel to reduce catalytic effects of the pollutants and is rated to operate at 300 psi pressure.

Next quarter plans include fabrication, installation, and check out of the sample collection system at atmospheric and elevated pressures, and initial collection of final test data at atmospheric conditions.

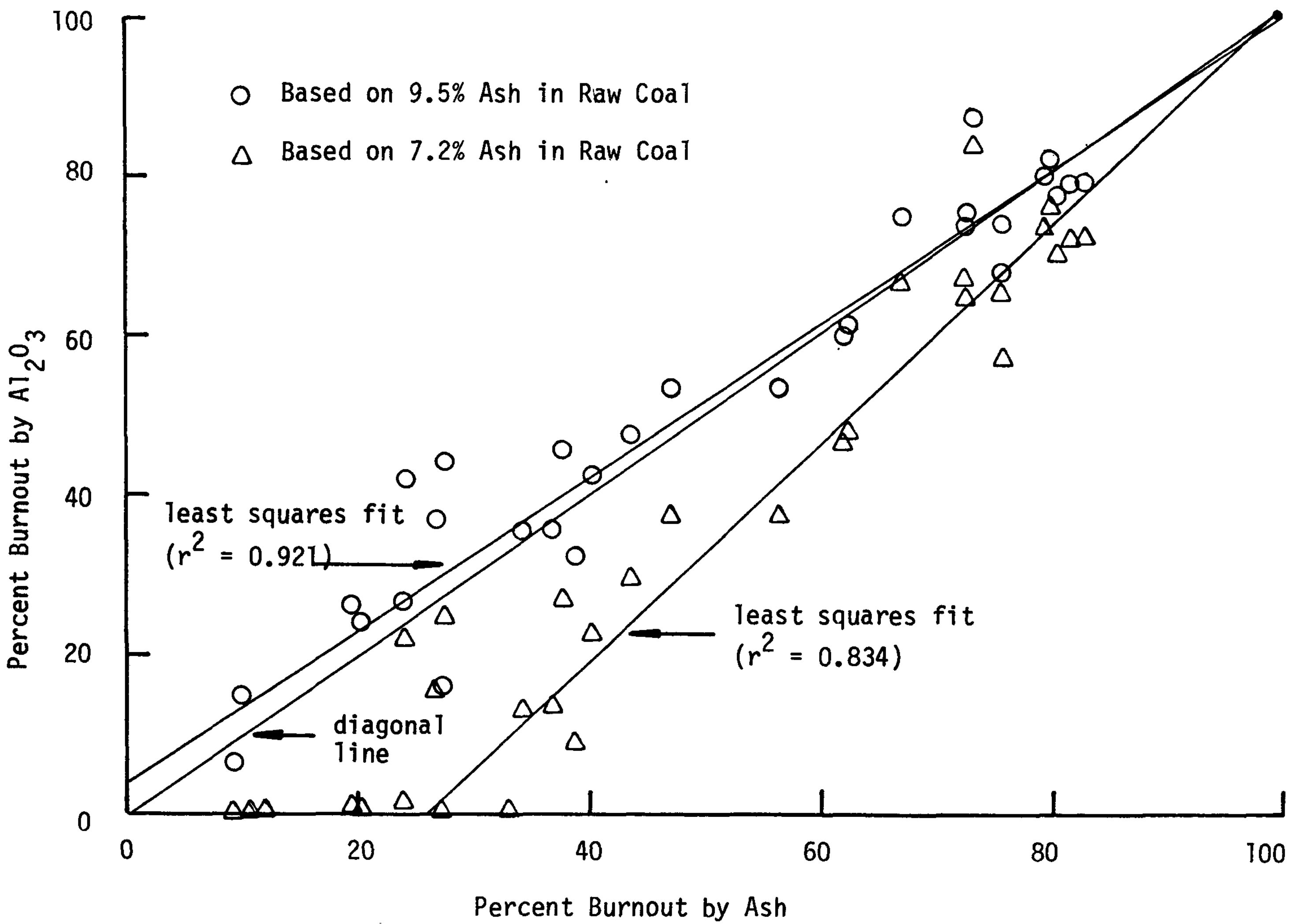


Figure 5. Comparison of Burnout as Calculated by Al_2O_3 and Ash.

Table 4

Preliminary Sample Results

Probe location: Centerline at 8 1/2" aft of exit

Amt. coal collected: 1.7 grams

Sample time: 90 seconds

Char Analysis

% Volatiles:	38.9
% Ash:	9.9
% Burnout:	
Based on Ash	14.5
Based on Al_2O_3	14.6

Liquid Analysis (ppm in gas)

CN^-	1 ppm
NH_3	.5 ppm

Gas Analysis (molar %)

O_2	16
N_2	56
CO_2	21
CO	6
H_2	trace
C_2H_6	trace

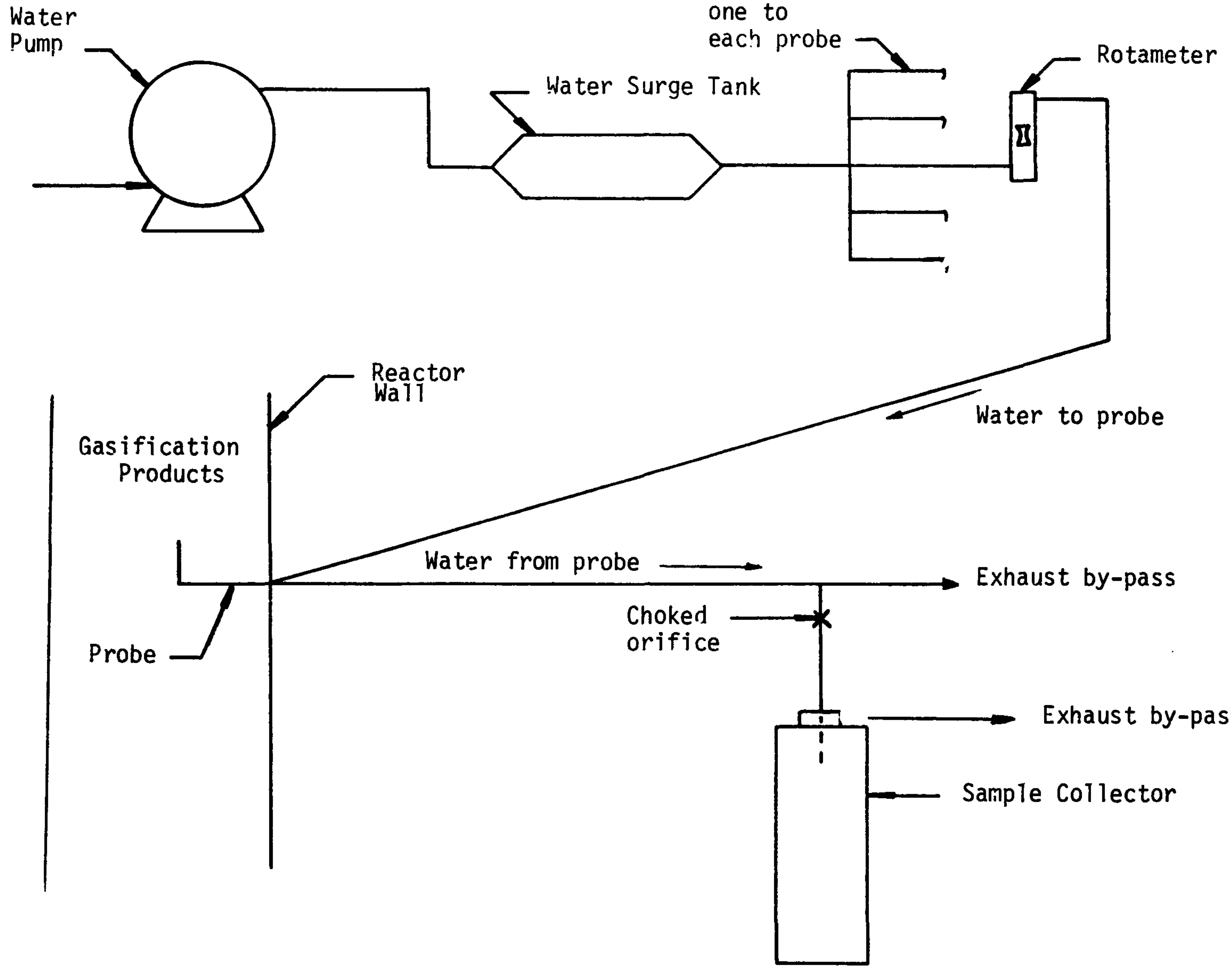


Figure 6. Schematic of Sample Train.

One-Dimensional Coal Gasifier Model Development

The one-dimensional model development was completed during the previous study. The code has been applied to several combustion and gasification systems and reported previously (7).

During this report period, the code has been applied to several more cases which resulted in improvements in the efficiency of the computations themselves as well as verification of applicability to a wide variety of conditions.

Model efficiency and performance has been improved in several areas during the application of the code to the different furnace or gasifier calculations. For example, severe numerical stability problems were encountered during an attempt to make model predictions for the BYU Rate Resolution Combustor in which the particle size distribution had a mass mean diameter of only 20 μm. In this particular case, the small particles burn out relatively early. After burnout the reaction rate disappears and the energy of the system only changes due to heat transfer effects such as radiation and convection to the reactor wall, conduction between particle and gas and particle-particle radiation within the reactor. A tight coupling is observed in the particles and gas energy differential equations (7), through the gas-particle conduction term resulting in a stiff differential system. Different methods were examined to resolve this stiffness in the most efficient manner. The pseudo steady-state approximation (pssa) for stiff differential systems (15) was found to be the most efficient. This assumption is invoked only after reaction rates become negligible and stiffness is encountered. By using this same approach, solution time for all calculations with the code has been reduced significantly.

Another example of code improvement was made during computations of the 5 ST/hr, DOE Bi-Gas entrained gasification system. In this calculation, very heavy particle loading resulted in difficulties with the radiation treatment. The optical depth was so short that conventional techniques required extremely small step sizes. Improved efficiency was achieved by treating radiation as a diffusion process for such systems (16). Subsequently, this option was successfully implemented.

In addition to computations previously performed and reported (17) and those already mentioned, the one-dimensional model was applied to the Coates Gasifier (18) during this report period. For this prediction, comparisons with measurements at the reactor exhaust were possible and excellent agreement between theory and measurement was observed.

During this report period, application of the model to industrial equipment was continued by completing three calculations on the first stage of a Babcock and Wilcox staged combustor. In this design the first stage is fuel-rich and some gasification is observed.

Work is also being concluded on the study to determine relative trade-offs resulting from variations in controllable parameters, and the sensitivity of the model to various input parameters. In particular studying the effect of the mixing and recirculation parameters on model predictions, and the effect of particle size distributions. This work seem to indicate mixing to be of secondary importance to heat transfer effects. Particle size effects seem to be of major significance.

Generalized Multi-Dimensional Model

Incorporation of the Probability Density Function (PDF) formulation into the two-dimensional code to describe diffusion-limited gas-phase combustion has also been completed and tested. Two independent models of different accuracy were developed to test the results. The PLOT program has also been implemented, and has been extended to include the PDF model. Plots of the finite-difference equilibrium and PDF solutions will be produced in the near future.

Work on PSI-cell development is continuing in consultation with C.T. Crowe. Development of QRAD has progressed as far as possible, given the severe lack of fundamental physical parameters available, even after exhaustive literature search and consultation with leading radiative heat transfer authorities. Plausible assumptions and simplifications have been established, subject to revision during validation tests in conjunction with experimental results.

PLANS FOR NEXT STUDY PERIOD

- Complete testing in the Cold Flow Test Facility with nonparallel injection in the presence of recirculation.

- Install back pressure regulator and check out gasifier at elevated pressures.

- Calibrate coal feeder for pressures in the range of interest.

- Install complete probe bank and sample collection system.

- Initiate cold-flow and reacting test programs at elevated pressures and obtain first final data results at atmospheric pressure.

- Continue testing of coal/oxygen/steam flames in the gasifier and obtain final test results.

- Continue the parametric study and the application of the one-dimensional code to industrial equipment.

- Continue the development of the generalized multi-dimensional code.

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