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MIXING AND GASIFICATION OF COAL IN ENTRAINED FLOW SYSTEMS

Quarterly Technical Progress Report No. 2
for the Period 1 July, 1977 to 30 September 1977

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NOTICE

FOREWORD

This report summarizes technical progress accomplished during the second report period of a two-year study being conducted for the Energy Research and Development Administration (ERDA) under contract No. EF-77-S-01-2666. This work period was 1 July 1977 to 30 September 1977. 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 ERDA.

Graduate and undergraduate students who have contributed to the technical progress and to this document were John Baardson, Rick Guercio, Stanley Harding, Don Leavitt, Jerry Sharp, Douglas Skinner, Philip Smith, and Scott Woodfield. Mr. James Hoen, Supervisor of the Research Machine Shop, has provided assistance in design and construction of reactor components. Michael King, Elaine Alger, and Scott Folster 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 accomplished during the second 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 first initiated in November 1974.

During this report period, eight additional cold-flow tests were conducted using an intermediate-size test chamber. Results verify the mixing chamber size is a secondary factor in controlling gas-particle mixing rates. Modification of this facility to permit nonparallel injection with recirculation was initiated.

The basic gasifier facility was completed during this past quarter and gas flames were ignited and stabilized on several occasions. Difficulties in obtaining uniform coal feed rates were encountered and alteration of the coal feeder was initiated to resolve these difficulties. Design and fabrication of a prototype of the sample train for removing gas-coal samples from the gasifier was also completed and is being tested. It was also shown that water does not alter coal or char samples but does dissolve some of the soluble ingredients in ash.

Application of the one-dimensional computer code to entrained gasifiers was initiated. Two computations for the laboratory gasifier illustrated the importance of the mixing process and showed that char-CO_2 reactions are slow compared to devolatilizaton and oxidation of the volatiles.

Integration of general gasifier computer model components was continued. The technical basis of the model was improved by accounting for micromixing processes. Sample computations were completed for the laboratory gasifier. It is anticipated that test work for coal-steam-oxygen flames will be initiated during the next report period.

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 crisis 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, bench-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 Furnace 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 ERDA/EPRI studies. Compare the model predictions to the experimental results.

Technical Approach

In order to accomplish the tasks outlined above, an entrained flow reactor has been designed and constructed. The reactor has been designed to operate at a peak pressure of 2000 kPa (20 atm). The high pressure reactor has been developed principally to study entrained coal gasification processes at elevated pressures, and has been constructed using funds from this study. The reactor 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 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-quench probes are required 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 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 investigated.

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

This model has a limitation in comparing with test results of Task 2 above, in that it does not allow prediction of radial variation of properties inside the reactor, while the data do provide both axial and radial distribution 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 development of more complex models.

During an independent study sponsored by EPRI (6), work was initiated to develop a generalized, multi-dimensional model of coal gasification processes. Many of the restrictions inherent in the one-dimensional model would thus be removed. During Phase 2, development of this generalized model will be continued under ERDA 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.

The previous cold flow tests with the expanded mixing chambers had indicated that the enhanced mixing with the smaller expanded chamber was as great as with the larger chamber. During this report period, a set of eight additional tests was performed with an intermediate sized duct to determine if there was an optimum size duct and if the intermediate chamber would enhance the mixing more than either the small or large chambers. These test results showed that in general, the greatest mixing occurred with the smallest expanded chamber. Modifications of the test facility were initiated in order to permit measurement of mixing rates with nonparallel injection and recirculation. Also, a paper was prepared for publication based upon recirculating flow test results.

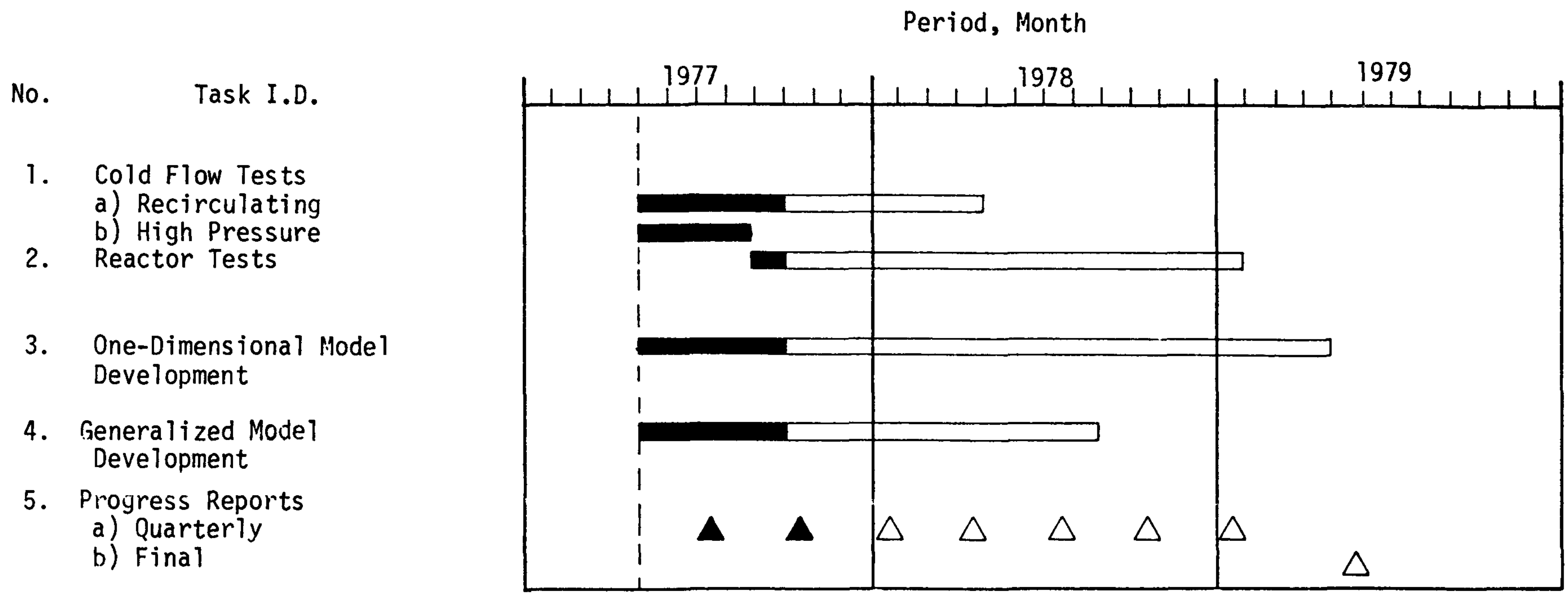


Figure 1. Summary Chart of Phase 2 Research Activities.

Task 2. Reactive Flow Tests and Analysis.

During the reporting period, the laboratory gasifier ignitor was designed, constructed, installed and tested. A gas flame was ignited and stabilized in the gasifier several times and no difficulties were encountered in lighting and sustaining methane-air or methane-oxygen flames. Wall temperatures in excess of 1200°K were achieved after 5 to 10 mintues of operation.

The steam boiler installation was completed and initial operation was begun. Initial attempts to introduce steam into the gasifier caused extinguishment of gaseous flames. It is expected that operation with coal and higher operating wall temperatures will solve that problem.

Problems were encountered with the coal feeder. Dumping on start up and shut down, and air entrainment effects have prevented reliable calibration of the feeder. Modifications to the feeder are being implemented in order to circumvent these problems. These modifications are based upon suggestions obtained from a recent ERDA-sponsored conference in Coal Feeding Systems.

The prototype sample train for the gasifier tests has been assembled and check out tests were begun. A nylon copolymer sample envelope has been placed inside the steel collection cell to allow full recovery of the gas, liquid and solids present. The nylon was selected because of its low permeability to the expected gas products. Actual collection tests in the gasifier are expected during the next quarter.

Task 3. One-Dimensional Coal Gasifier Model Development and Application.

The one dimensional model was applied to the more complex coal gasification problem during the report period. Further debugging of the code was required but predictions were made for the gasifier under two specified conditions: a totally premixed situation at the reference gasifier operating conditions (7), and a reference operating situation (7) where the mixing rates of the primary, secondary, and recirculating streams were arbitrarily specified. These preliminary results indicate that the gasification in the laboratory reactor is strongly affected by the mixing and recirculation processes.

Task 4. Generalized Furnace Model Development.

Subcontract work on this task was initiated at the University of Utah on June 1, 1977, as a contination of work previously sponsored by EPRI (18). This activity is directed toward the modular construction of a large-scale computer code which will make theoretical predictions of the turbulent mixing and reaction of coal-gas mixtures in complex reactor geometries.

Major revisions to the code component dealing with chemical reaction (CHEM) are being made which will remove a serious lack of capability of the generalized model to deal with fluctuating flow chemistry interaction. Some of the links between model subcomponents have been completed and all binary links will be demonstrated and first attempts at complete linkage will be initiated during the next reporting period. Authorization has been obtained to use the CDC 7600 computer at Lawrence Berkeley Laboratories for the fully-linked runs.

Task 5. Progress Reports.

This report represents the second quarterly report on the current ERDA contract. One technical paper (11) has been prepared for journal publication during the reporting period. The technical paper was based on results obtained from the cold flow mixing tests in the presence of recirculation.

DETAILED DESCRIPTION OF TECHNICAL PROGRESS

Cold Flow Tests Without Recirculation

During this report period, eight cold flow tests were performed, corresponding to test conditions I (reference - gas only) and II (reference with 40% solids loading) of the previously reported test schedule (12). Comparisons of these tests with tests run previously on this facility (13) are shown in Figures 2 and 3. The previous tests used a small (205 mm diameter) and a large (343 mm diameter) recirculation chamber, while the current tests used a medium-sized (260 mm diameter) recirculation chamber.

Previous tests had shown that the enhanced mixing with the small expanded duct was nearly the same as with the large expanded duct. This suggested that there may be an optimum duct size. The purpose of these additional eight tests was to determine if an optimum existed and if so what geometry was optimum. The gas decay data of Figure 2 and 3 show that the rates of mixing are greatest for the small mixing chamber, as was the case with the particles. However, the medium size mixing chamber appears to give the poorest rates of mixing for gases. This latter result may be questionable because of possible gas analysis problems.

The particle decay data of Figure 3 show that the rate of mixing of the particles increases with increasing mixing chamber diameter. The greatest mixing occurred with the small mixing chamber, which has a ratio of mixing chamber diameter to secondary exit diameter of 2.05.

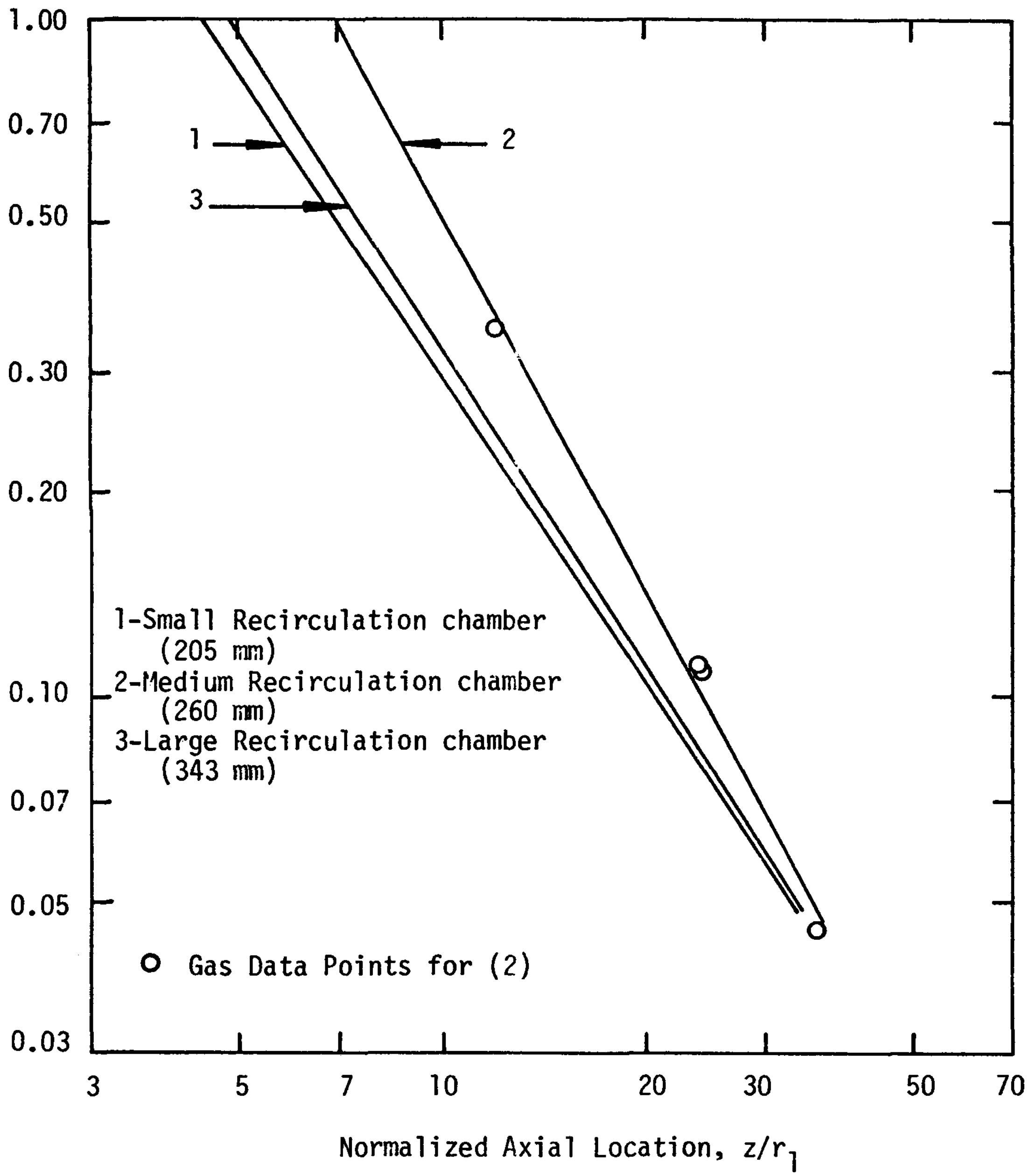


Figure 2 Comparison of Axial Decay Data of Flow Condition I for the Cold Flow Recirculating Tests.

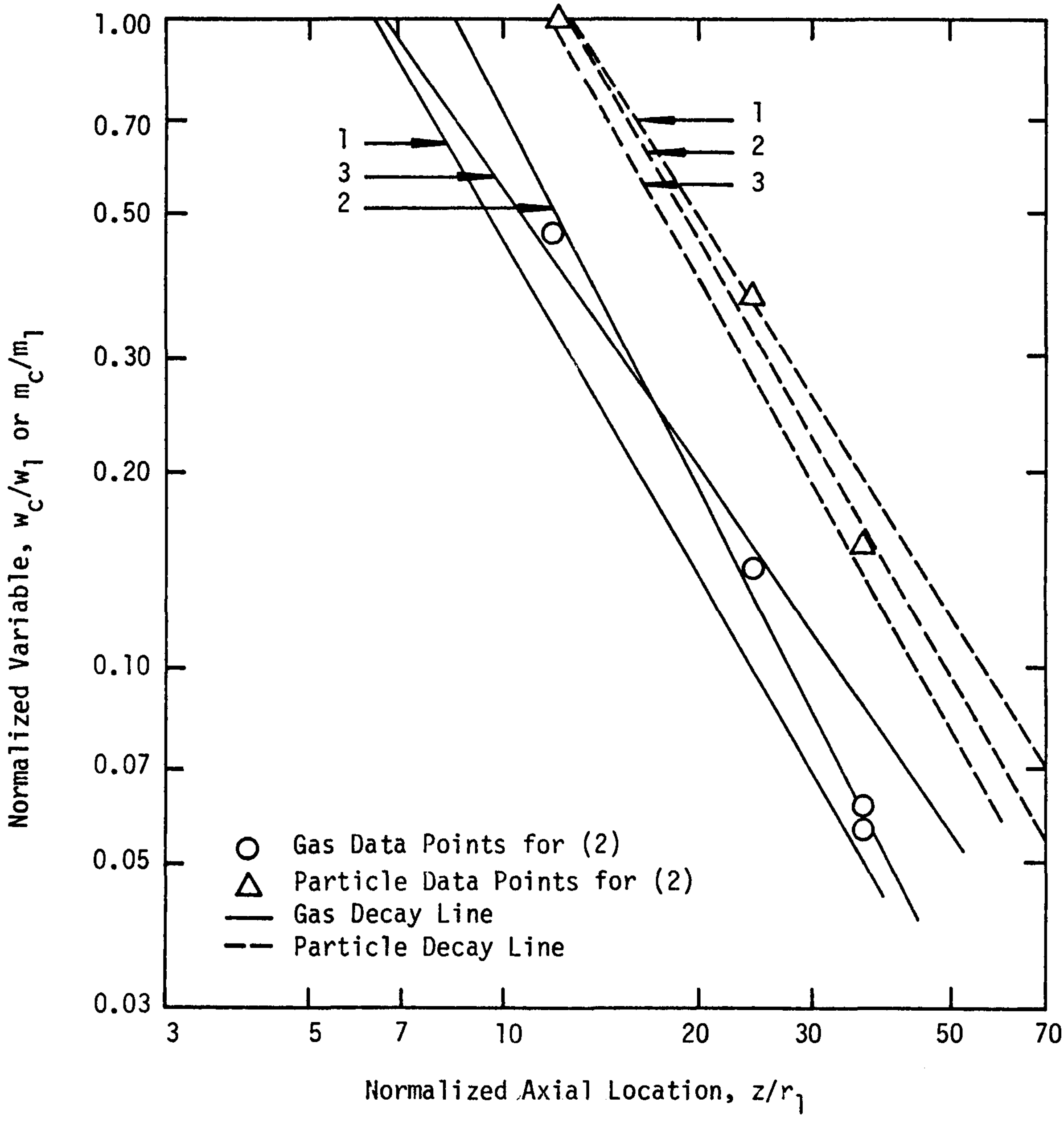


Figure 3 Comparison of Axial Decay Data of Flow Contition II for the Cold Flow Recirculating Tests.

Fabrication was begun on a modification to the cold flow facility which will enable the use of the nonparallel secondary injection collar used by Memmott (19) with the recirculation chambers presently in use. Fabrication of this connection piece is expected to be completed within two to three weeks. An electrical problem in one of the instrumentation recorders used on the cold flow facility has delayed testing. Repairs are underway at present to correct these problems and testing will resume shortly.

Plans for the next quarter are to resolve any questions concerning the gas mixing data previously discussed and to continue with the test program outlined in the previous report.

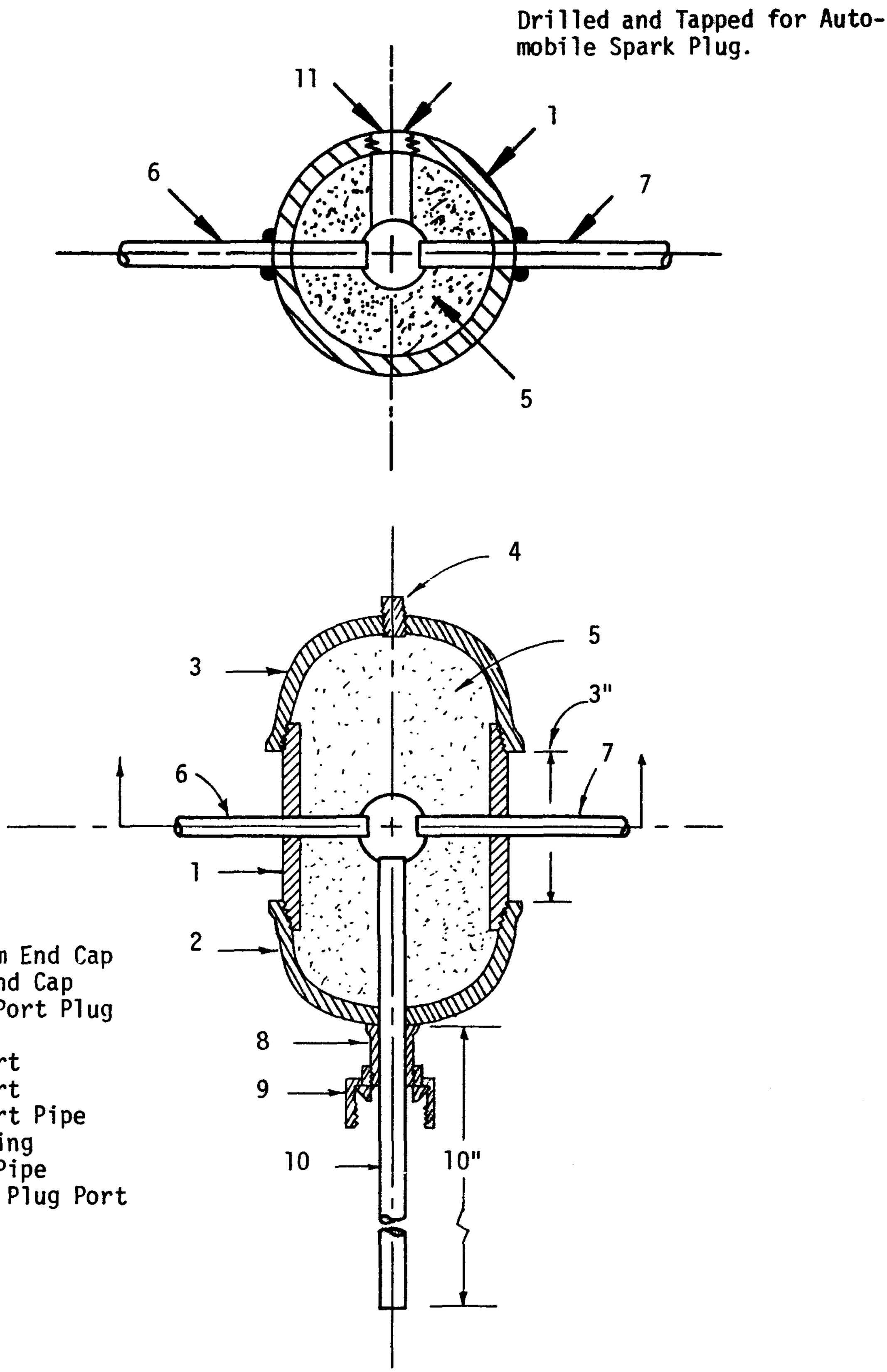
Reacting Gasification Tests and Analysis

Technical Visits. Dr. Hanks has attended two different technical programs dealing with coal feeding. He attended the US ERDA-sponsored Conference on Coal Feeding Systems held at the California Institute of Technology on June 21-23. The purpose for attending this meeting was to seek information which might help to resolve a problem which had developed with the high pressure coal feeder. He also attended the AIChE Today Series special course on Storage and Flow of Solids in Denver, Colorado on August 29-30. This special two-day intensive course was offered by Dr. A.W. Jenike and Dr. J.R. Johanson. One full day of the course dealt directly with problems pertinent to the coal feeder and Dr. Hanks was able to discuss our feeder directly with Dr. Johanson.

A visit was also held with Dr. Ralph L. Coates at the Eyring Research Institute concerning their coal feeder which is similar in design to ours. This meeting likewise resulted in some ideas about how to change the feeder and associated piping. As a result of these conversations, a number of design changes for the feeder were conceived and are now being implemented.

Test Facility. During the past quarter the gasifier igniter, shown in Figures 4 and 5 was designed, constructed, installed and tested and is now functional. The igniter body consists of a short piece of 4 inch, schedule 80 steel pipe with caps on each end. The core is lined with castable ceramic except for the entry ports. Stainless steel tubes admit H_2 and O_2 so that the streams directly impinge upon one another. Ignition is obtained from a spark plug mounted in the plane of the inlet pipes. Hot exhaust gases leave by way of the ceramic tube in the bottom of the ignitor, and pass through the tube into the gasifier where they ignite methane-air-oxygen mixtures for preheating purposes.

The igniter which is attached to the gasifier head and supported by a steel pipe and union coupling (Figure 5), is also externally plumbed to allow methane to be fed through it to the gasifier.



No.	Part
1	Body
2	Bottom End Cap
3	Top End Cap
4	Fill Port Plug
5	Liner
6	O_2 Port
7	H_2 Port
8	Support Pipe
9	Coupling
10	Exit Pipe
11	Spark Plug Port

Figure 4. ERDA Gasifier Igniter Assembly.

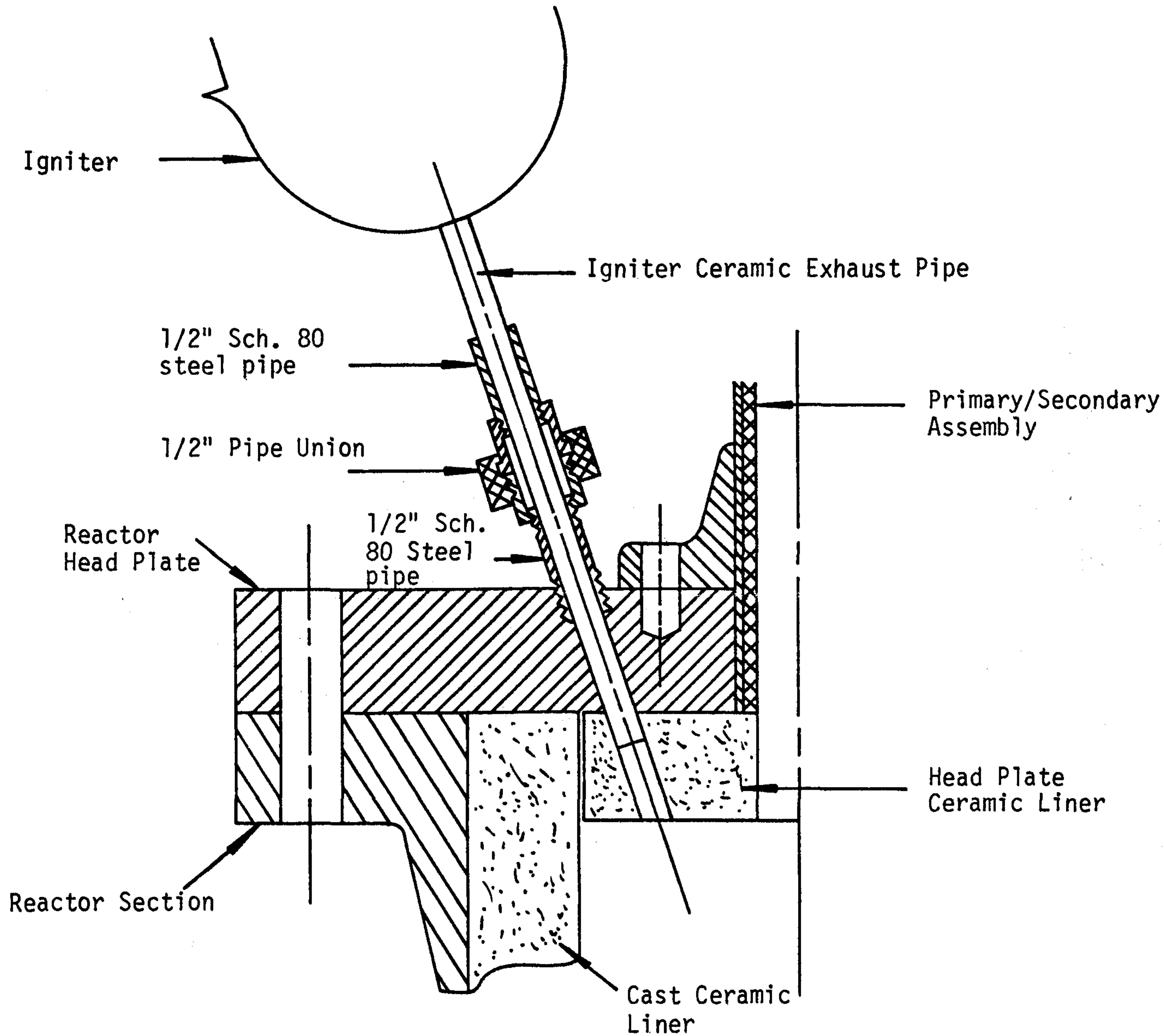


Figure 5 Igniter Installation in Gasifier.

During this quarter, gas mixtures have been ignited and stabilized several times in the gasifier. It has been demonstrated that inside wall temperatures in excess of 1200°K can be achieved in a matter of 5-10 minutes. No difficulties were encountered in lighting and sustaining methane/air/oxygen flames using this ignition system.

The steam boiler vessel was chemically cleaned to remove any oils or other undesirable materials and the boiler and associated flow control loop were checked out. An attempt was made to introduce steam into a methane-oxygen flame, but due to low wall temperature this caused extinguishment of the flame. Check out testing with steam will be continued during the next quarter.

Feeder Design Changes. A significant amount of time was spent on attempting to calibrate the coal feeder. Dumping of coal on startup and shutdown due to pressure imbalances continued to be a problem. Also, different entrainment air flow rates were shown to have a pronounced effect on the coal delivered at a given feed setting. A major effort was begun to find solutions to the coal feed problems. The trips by Dr. Hanks, discussed earlier, were part of this effort.

The erratic and uncontrollable feeding of coal under entrainment air-flow conditions has been traced to two major sources. The feed tank apparently operates in the funnel flow rather than the mass flow mode (14), giving irregular coal feed rates. Also the Acrison open core augers being used do not draw uniformly and are very sensitive to pressure differentials, readily permitting pressure driven flow of fluidized coal in either direction.

In an attempt to prevent funneling of the coal bed, a stirrer has been designed and constructed. Also, variable-flighted, solid-core auger screws have been designed and are being constructed. These improvements should be operative shortly and will be discussed in the next quarterly report. The plans for next study period are to complete modifications to coal feeder and calibrate, stabilize coal/-flames, complete check out of sampling probe and collection system under reaction conditions, and make preliminary high pressure check out runs.

Coal Analysis Tests have been conducted to determine the volatility of ash at elevated temperatures in order to correctly use ash as a particulate tracer. These tests have been completed up to 1750 K and were reported in the last program report. It was shown that ash is partially volatile but that iron, a key ash component, remains unaffected at the higher temperatures. However, testing at even higher temperatures is needed to accurately quantify the effects on both ash and iron compositions at reactor operating conditions. Because of the limitation of the muffle furnace the use of an alternate furnace capable of achieving at least 2100°K is being considered.

Tests were also conducted to determine the effects of probe quench water of varying pH on the coal, char, and ash. These tests were completed during the study period and are summarized in Table 1. Because of the relatively low recovery percent of the ash using a 0.8 μm mesh filter, further tests were done using a 0.025 μm mesh filter. However, no improvement was shown. It therefore seems apparent that certain ash compounds are soluble in the water solution. Based on the results from the U.S. Geological Survey on ash composition shown earlier in Ref. 7, about 9% to 10% of the ash is probably soluble, as summarized in Table 2.

To confirm this supposition, analyses for various elements such as K, Na, Ca and Mg in water solutions are being conducted using an atomic adsorption analyzer, both before ash has been put in and after ash has been filtered out. Results are expected to be obtained during the next quarter.

Sample Train. During this quarter fabrication of the proposed sample train was accomplished and check-out tests were done. Preliminary results are encouraging, but minor adjustments have been made. Nylon 6/6-6 copolymer sample bags have been placed inside the steel collection cell in order to facilitate recovery of all gas, liquid, and solids present and prevent contamination of the sample by the steel cell. Nylon was chosen because of its low permeability to the combustion gas products.

During the next quarter, further checkout tests are anticipated and the use of the sample train under reacting conditions will be done.

One-Dimensional Coal Gasifier Model Development and Application

Model Basis. The basis for a computerized model for predicting characteristics of entrained coal gasifiers was developed during Phase 1 of the previous study (7). This model uses the integrated or macroscopic form of the general conservation equation for a volume element inside the gasifier. A summary of key model assumptions and conditions was given in Ref. 7. The following aspects of pulverized coal gasification have been included in the model:

(1) mixing of primary and secondary stream;

(2) recirculation of reacted products;

(3) pyrolysis and swelling of coal;

(4) oxidation of the char by oxygen, steam and carbon dioxide;

(5) conductive/convective heat transfer between the coal/char particles, gases and reactor wall;

(6) variations in composition of inlet gases and solids;

(7) variation in coal/char particle size;

Table 1

Quench-Water Effects on Coal, Char and Ash

	% Recovered	% Volatiles Change	% Ash Change
COAL	99.0	0[1]	-4.4[1]
CHAR	98.2	NA[3]	NA
ILLINOIS CHAR	98.6	0[2]	-7.5[2]
ASH	94.9	---	---

[1]% difference from ASTM proximate analysis of original coal.

[2]% difference from ASTM proximate anlaysis of screened char

[3]NA = Not available.

Table 2

Ash Solubility

Compound	% of Ash+
Soluble in Water	
Na_2O	4.3
SO_3	3.5
P_2O_5	1.
K_2O	0.7
	9.5
Insoluble in Water	
MgO	1.1
Al_2O_3	17.0
CaO	6.5
SiO_2	48.0
TiO_2	0.9
MnO	0.05
Fe_2O_3	3.8
	77.4

+From U.S. Geological Survey Analyses of Test Coal (15).

(8) oxidation of the coal pyrolysis products;

(9) radiative interchange among particles and with the reactor wall.

Differential mass and energy balances were developed for particle and gas phases and were summarized in Ref. 7. 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;

Status. During the preceding report period, development and debugging of the computer code had been completed, and predictions had been made for a simplified combustion system. During this report period the code was applied directly to the gasifier conditions which will be used in the laboratory experiments of this study. This direct application uncovered several areas in the code where further debugging was required. This task was accomplished and predictions were made for the gasifier operating under the two specified conditions listed below.

(1) Input parameters were from the base case for the laboratory gasifier (Flow Condition 1 of Ref 7 p. 47); however, the primary and secondary streams were assumed to be completely premixed and reacting in plug flow. This allowed examination of reactor dynamics without having to specify detailed mixing parameters for either recirculation or primary and secondary mixing.

(2) A more realistic calculation followed in which mixing rates of primary, secondary and recirculating streams were input. Results of these calculations are shown in Figures 6, 7, and 8. The input parameters for this prediction were, as in the premixed case, Flow Condition 1 of Ref. 7 p. 47. The results of these calculations indicate that pyrolysis and subsequent oxidation of the pyrolysate is very rapid. Oxygen is depleted in this devolatilization phase and the oxidation of the char with steam and carbon dioxide follows slowly. The calculations indicate that with a single coal particle size of 60 um, char burnout is not quite complete in the gasifier of 112 cm length. The results of these two calculations indicate that gasification in the laboratory reactor is strongly affected by the

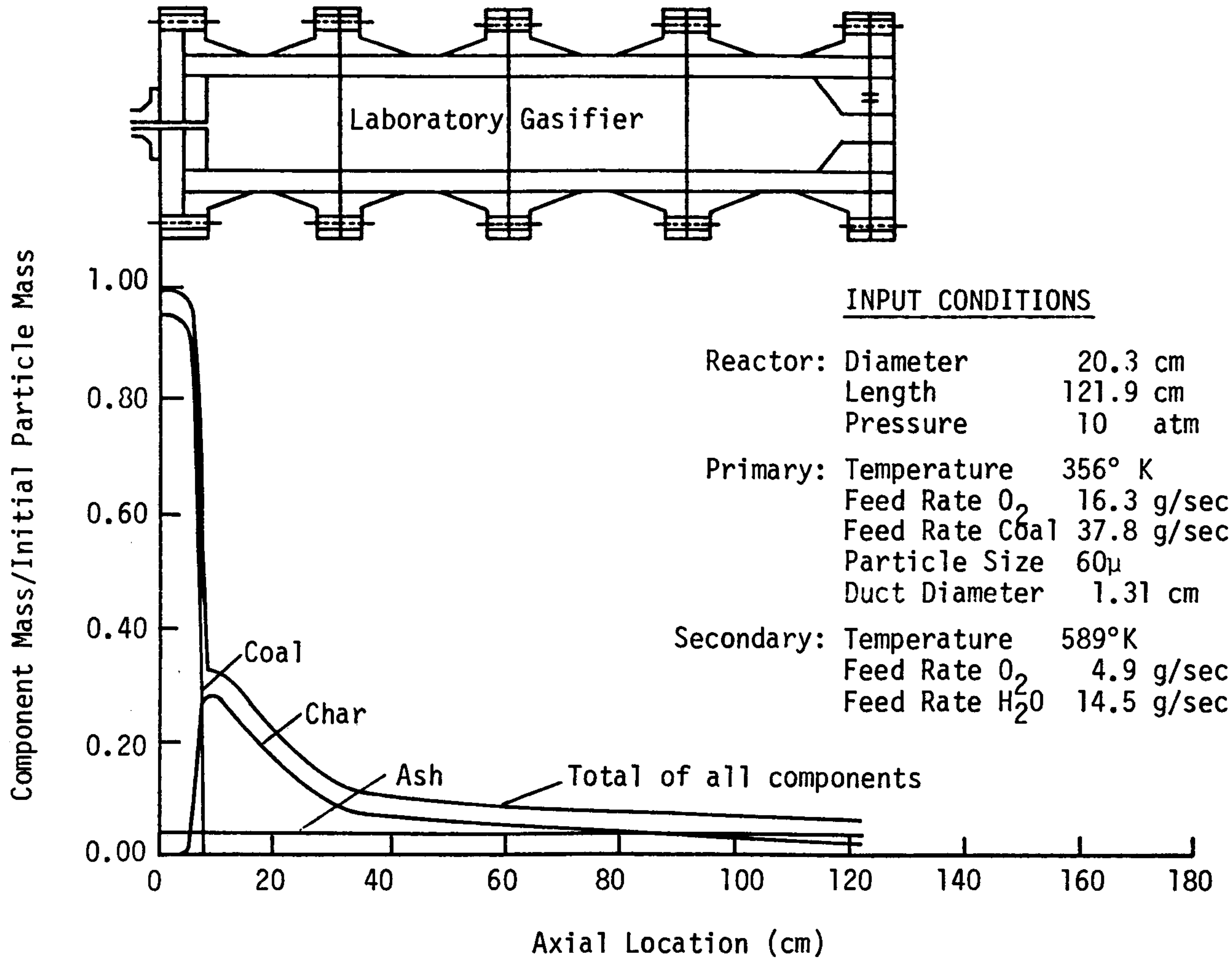


Figure 6. Particle Mass History.

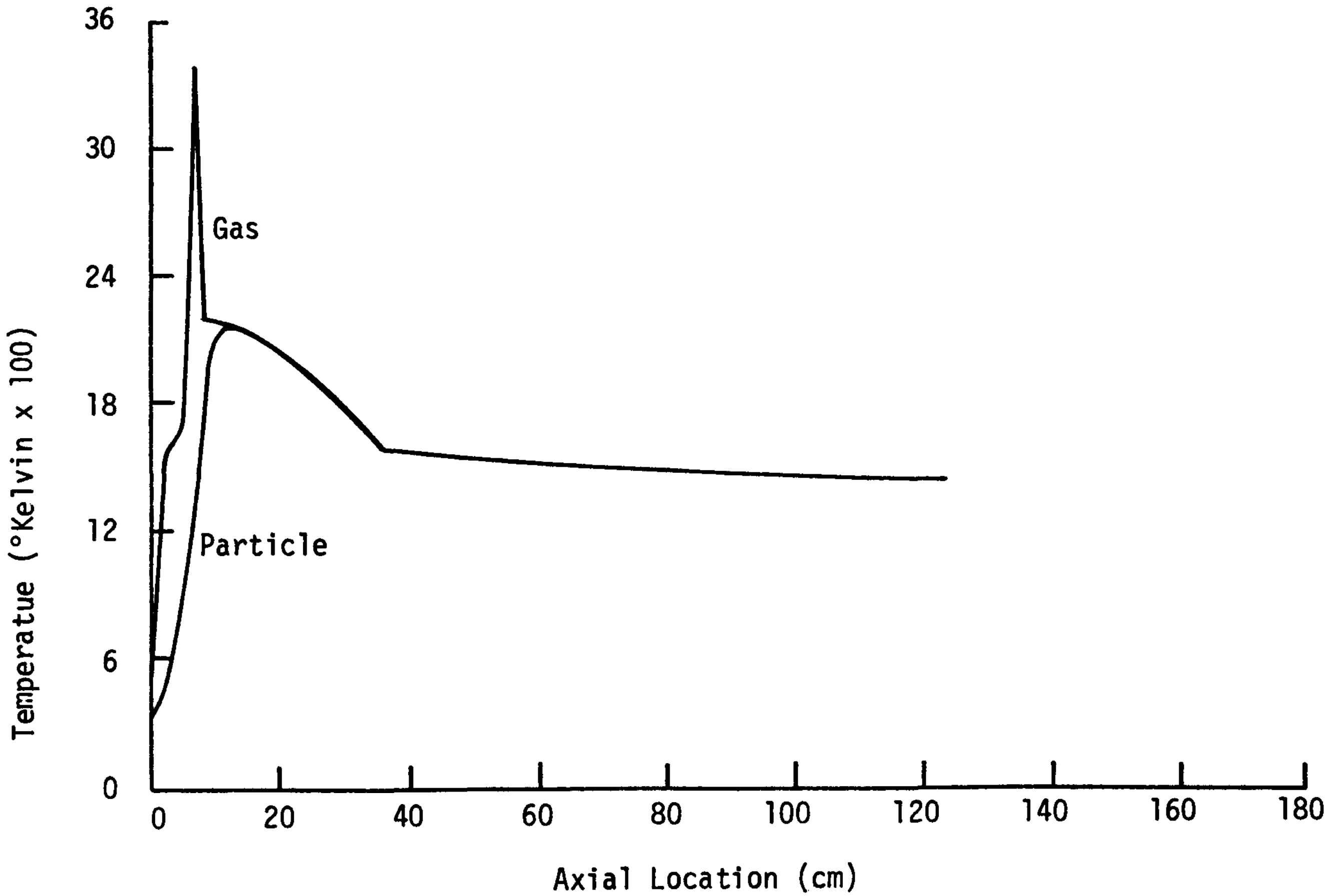


Figure 7 Particle and gas temperatures.

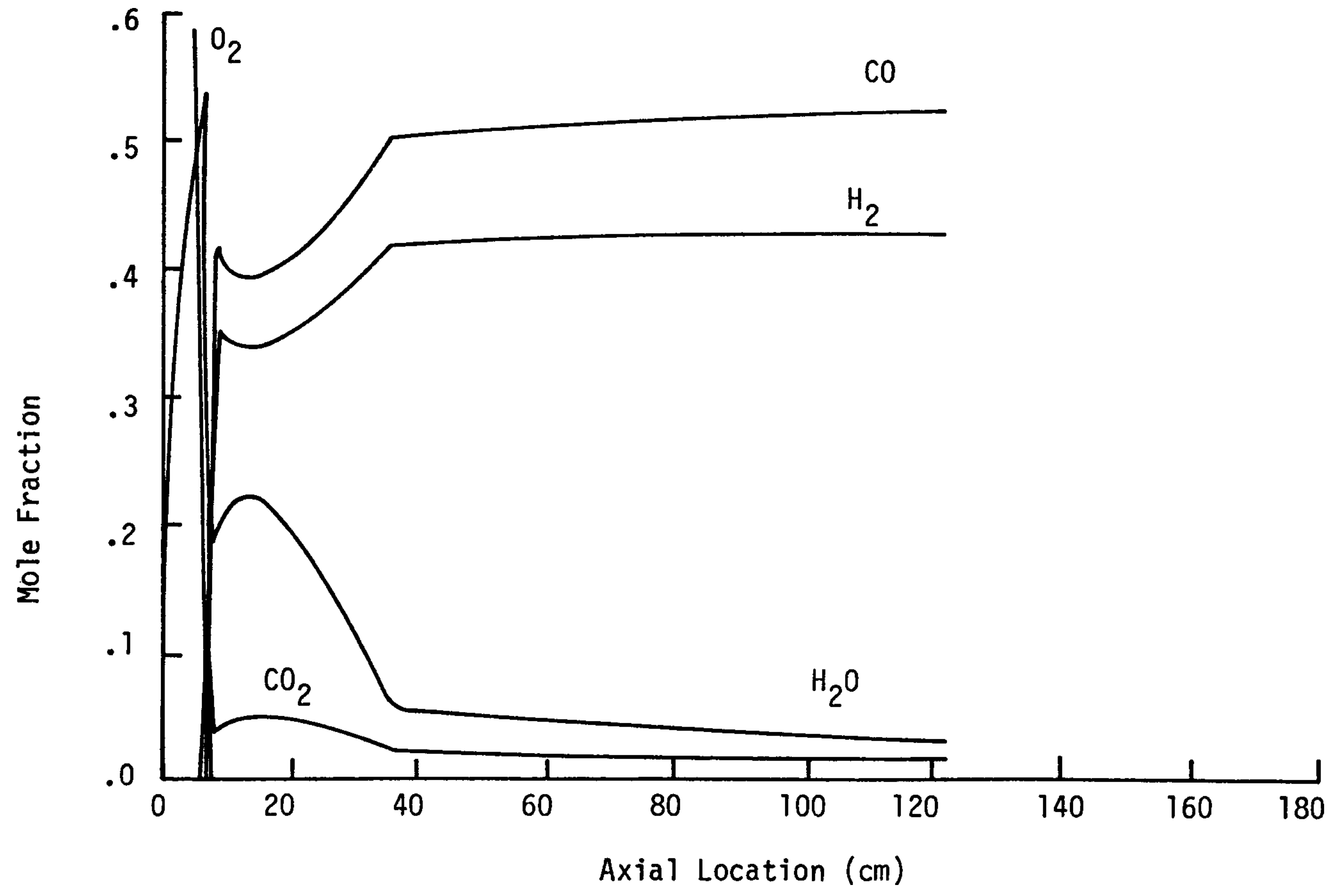


Figure 8 Gas specie mole fractions.

mixing and recirculation processes.

Another accomplishment of this report period has been to increase the efficiency of computing time. Increased efficiency in the equilibrium calculations have decreased computing time by more than a factor of 2. A typical converged solution now requires 5-15 minutes on a relatively small DEC-10 computer, which is equivalent to 0.5-1.5 minutes CPU time on a CDC-7600 computer.

Plans. There remains only one aspect of the one-dimensional model development which has not yet been tried at least once. Up to now all calculations have been done assuming a uniform size of all coal particles. During the next quarter development will focus on multiple particle-phase calculations. Finally, an extensive parametric study will be conducted to determine relative trade-offs resulting from variations in controllable parameters.

Generalized Furnace Model Development

Work on this subcontract was initiated at the University of Utah by J.J. Wormeck, D.T. Pratt and A.J. Varma, on June 1, 1977. About one month was required for orientation of Dr. Wormeck to the UNIVAC 1108 computer operating system, and for implementing the program sub-elements developed at BYU under prior EPRI sponsorship (16-18).

Briefly, this activity is directed toward modular construction of a large-scale computer code which will eventually be utilized for sensitivity analysis of physical parameters, scaling, and ultimately design of continuous, pulverized fuel gasifiers and furnaces. In addition to the main routine, which controls the linkage of program modules (SUBROUTINE subprograms), main subcomponents are (1) FLOW, (2) CHEM, (3) PSIC, (4) QRAD, and (5) COAL. In the order cited, these subelements solve the governing differential and algebraic physical model equations related to (1) turbulent gas-phase flow dynamics, (2) turbulent gas-phase chemistry and heat release, (3) dynamic interaction of turbulent flow with coal particle dynamics, (4) thermal radiation transfer between gas, walls and particles, and (5) physical chemical processes occurring within the coal particles, respectively.

Element FLOW has been 100% complete for some time. CHEM, previously completed at the level of infinite-rate or equilibrium chemistry, is now being expanded to include a capability for finite-rate micromixing with equilibrium chemistry. This extension is a major improvement over the infinite-rate micromixing, which was viewed as one of the major shortcomings of the model as originally proposed. It is anticipated that this extension will be 100% complete within the next reporting period.

The linkage between FLOW and CHEM (gas-phase only flow and chemistry) has been successfully implemented. QRAD is presently at about 80% completion. As mentioned in earlier quarterly reports on the EPRI-sponsored phase (16-18), this module required the most new work of the components. It was necessary to derive the governing "fourflux" model of radiative transfer from first principles, as it was discovered that no such reliable derivation existed in the literature. Sub-modules include the capability to compute only a two-flux model (neglecting radial transfer), and to consider either constant or variable properties of gas and particle cloud optical properties. Original work arising from the need to research this subject will result in two or more separate publications.

PSIC is being developed with assistance of Dr. Clayton T. Crowe of Washington State University, consultant to the project. While carefully reforumulating this approach to solid-gas phase dynamic coupling, several questions arose regarding treatment of both turbulent particle dispersion, and the formulation of coupling terms between the solid and gas phase energy equations. These questions are presently being resolved and it is expected that PSIC will be 100% complete within the next reporting period.

Linkage of PSIC and FLOW has been demonstrated, with a graphical output plotter package plot developed specifically for this application. Validation with cold-flow particle dispersion data discussed above will be attempted immediately following final resolution of remaining questions in the PSIC formulation.

Element COAL contains a proposed model for treatment of an individual coal particle subjected to a given chemical, thermal and radiative environment. Formulation is approximately 90% complete, and should be complete within the next reporting period.

During the next reporting period, binary linkage of elements will continue, and will be validated whenever appropriate data exists. It is expected that first attempts to link all modules will occur during the next reporting period, but this will not be attempted until all binary links have been satisfactorily accomplished. Permission has been sought and approved to use the ERDA-sponsored CDC 7600 computer at Lawrence Berkeley Laboratories for the complete linkage runs.

Figure 6 illustrates selected computations for the laboratory gasifier. Part (a) shows gas temperature profiles, (b) shows gas streamlines and (c) shows coal particle trajectories. These computations are preliminary, but illustrate the kinds of properties the code will predict.

OTHER ACTIVITIES

During August of 1977, Dr. Smoot and Dr. Hedman visited ERDA in Washington, D.C. to report on technical progress for this study. Dr. Smoot also presented a review of contract activities at the Annual ERDA-ERPI-NSF University Contractors Conference in Pittsburgh, Pa. August 25 and 26, 1977. A paper by C. Tice and L.D. Smoot was prepared for submission to the AIChE Journal, entitled "Cold Flow Mixing Rates with Recirculation for Pulverized Coal Reactors". Technical visitors to this laboratory during the report period included Mr. Robert Carr,

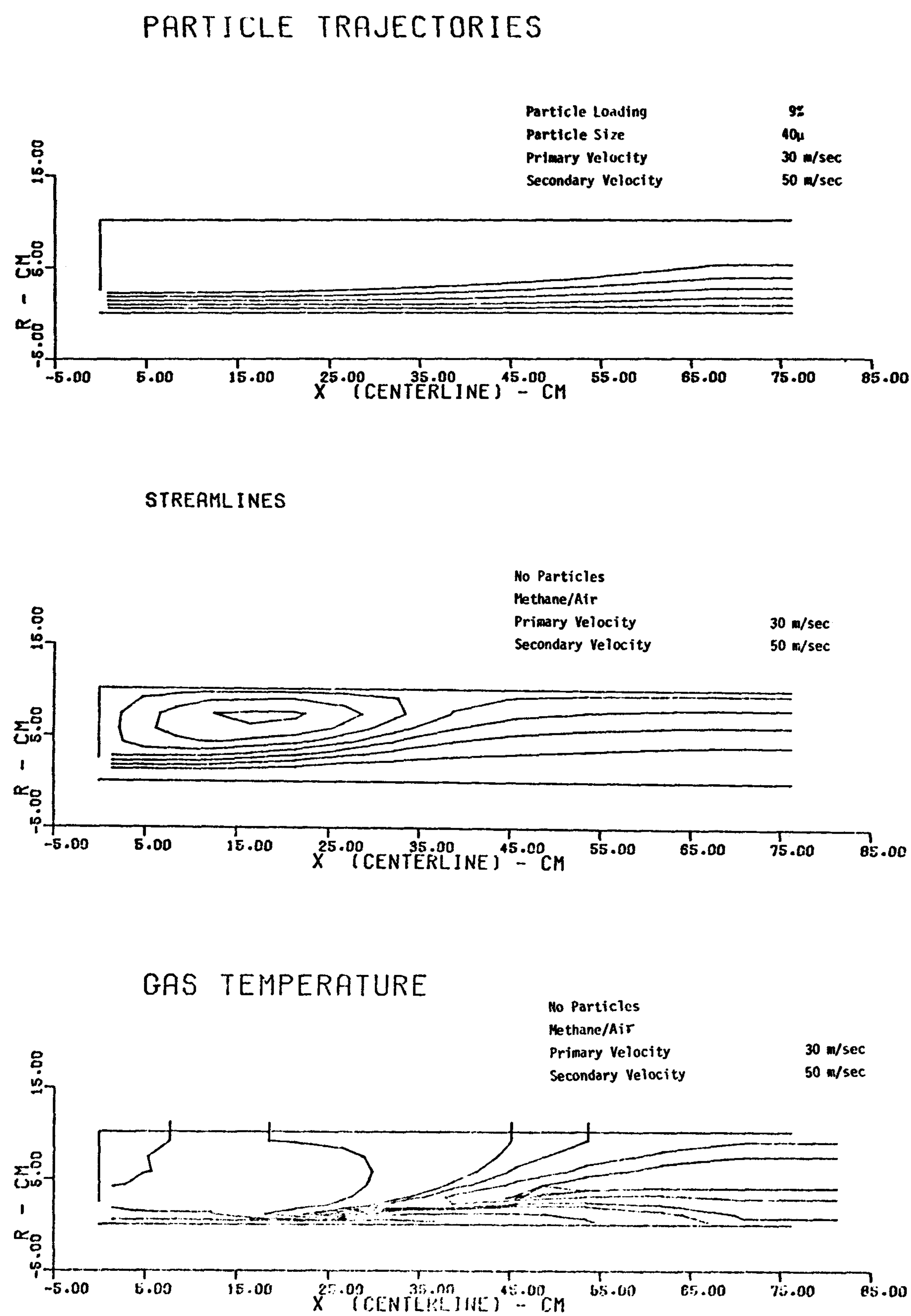


Figure 9 Preliminary Predictions Using Multi-Dimensional Coal Gasification Code

EPRI, Dr. Ed Kansa, Bureau of Mines, and Dr. C.L. Chen, Babcock and Wilcox.

PLANS FOR NEXT STUDY PERIOD

- Comlete revision to Cold Flow Test Facility, and initiate testing with nonparallel injection in the presence of recirculation.
- Resolve coal feeder problems and calibrate coal feeder.
- Check out sample train system.
- Stabilize coal/steam/oxygen flames in gasifier.
- Debug one-dimensional gasifier model for multiple particle sizes and initiate parametric gasifier computations.
- Complete extension of model to account for micromixing rates and continue integration of generalized model components.

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