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PREDICTION AND MEASUREMENT OF OPTIMUM OPERATING CONDITIONS FOR ENTRAINED COAL GASIFICATION PROCESSES

Quarterly Technical Progress Report No. 1, November 1, 1979—January 31, 1980

MASTER

By
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February 15, 1980

Work Performed Under Contract No. AC21-80MC14380

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DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

U. S. DEPARTMENT OF ENERGY

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ABSTRACT

This report summarizes work completed during the first quarter of a two-year study to predict and measure optimum operating conditions for entrained coal gasifications processes. This study is the third in a series designed to investigate mixing and reaction in entrained coal gasifiers.

A new team of graduate and undergraduate students was formed to conduct the experiments on optimum gasification operating conditions. Additional coal types, which will be tested in the gasifier were identified, ordered, and delivered. Characterization of these coals will be initiated during the next quarter. Hardware design modifications to introduce swirl into the secondary were initiated. Minor modifications were made to the gasifier to allow laser diagnostics to be made on an independently funded study with the Los Alamos Scientific Laboratory. A Master of Science thesis and a Ph.D. dissertation based on the previous Phase 2 study were nearly completed.

The tasks completed on the two-dimensional model included the substantiation of a Gaussian PDF for the top-hat PDF in BURN, the completion of a Lagrangian particle turbulent dispersion module. The reacting submodel is progressing into the final stages of debug. The formulation of the radiation submodel is nearly complete and coding has been initiated.

A device was designed, fabricated, and used to calibrate the actual Swirl Number of the cold-flow swirl generator used in the Phase 2 study. Swirl calibrations were obtained at the normal test flow rates and at reduced flow rates. Two cold-flow tests were also performed to gather local velocity data under swirling conditions. Further analysis of the cold-flow coal-dust and swirl test results from the previous Phase 2 study were completed for incorporation into a Master's of Science thesis.

FOREWARD

This report summarizes technical progress accomplished during the first quarterly reporting period of a two-year study being conducted for the U. S. Department of Energy (DOE)). This work period was 1 November 1979 to 31 January 1980. Work was accomplished under the direction of Dr. L. Douglas Smoot, principal investigator, and Dr's. Paul O. Hedman and Philip J. Smith, senior investigators. Dr. Surgit Singh is the program manager for DOE.

Graduate and undergraduate students who have contributed to the technical progress and to this document were D. Ronald Anderson, Vearl Beck, Thomas H. Fletcher, Scott C. Hill, Stephen Kramer, Don Leavitt, Guy Lewis, Ronald M. Orme, Wesley Pack Jr., Tracy D. Price, and F. Douglas Skinner. Mr. James Hoen, Supervisor of the Research Machine Shop, has provided assistance in design and construction of reactor components. Michael King, Elaine Alger, and Kathleen S. Hartman have provided technician, typing and drafting services.

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OBJECTIVE AND SCOPE OF WORK

Background

The large energy requirements of our country and the necessity of importing a significant fraction of our petroleum fuels have demonstrated the need to develop alternate energy sources. Nuclear, geothermal or solar energy may eventually meet part of this increasing energy need. However, with our present level of technology, we will not be able to supply all of the increasing demands economically from these sources. As a consequence, it is necessary to continue to convert energy from fossil fuels for a considerable time into the future.

A number of different types of coal conversion processes have been proposed, explored and are being developed to produce clean, economical supplies of gas and oil from coal. Several of these coal processes involve, either directly or indirectly, the injection of finely pulverized 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.

Considerable progress has been made by researchers in the BYU Combustion Laboratory in developing an understanding of the effects of mixing and reaction in entrained coal systems. Two experimental facilities have been developed--one designed for coal gasification at pressures up to 20 atm (1,2) and a second for coal combustion at atmospheric pressure (3,4). Both of these reactors are of sufficient scale to allow gas and particle samples to be taken locally within the reactors. These fully functional reactors provide unique experimental tools which can be used to conduct optimization studies or which can be used to determine the gasification or combustion rates of a given coal in a realistic environment.

Also, two computer codes have been developed which can be used to describe the operation of entrained coal reactors. The first code is a one-dimensional code which requires, as input, the mixing and recirculation rates between the primary and secondary streams, but which then describes coal heatup, pyrolysis or devolatilization and heterogeneous reaction of the char with the gaseous reactants. The second code is a generalized, two-dimensional model for turbulent, reacting systems which has been developed to the point where predictions for gaseous mixing and reaction can be made. The extension of the two-dimensional code to include coal pyrolysis and reaction is included as a part of this research program.

There is considerable process development work underway to develop new coal gasification, coal liquefaction and coal combustion hardware. However, there is very little work of a more fundamental nature directed toward understanding the basic reaction processes. A basic understanding of coal reactions is important in successfully developing these complex processes. In fact, over the years, several developing processes have not been successful, at least in part, because they lacked the fundamental data and techniques needed for optimum design.

This study, a continuation of a Phase 1 ERDA study (1) and a Phase 2 DOE study (2) on coal mixing and gasification in entrained systems, includes a parametric investigation of entrained coal gasification operating variables to optimize coal burnout (thermal efficiency), product distribution and pollutant formation. The program provides for completion of the two-dimensional gasification code by incorporating the coal pyrolysis, devolatilization and heterogeneous chemical reaction schemes which are currently functional in the one-dimensional code. The local properties measured inside the coal reactor will provide data to validate the two-dimensional code.

Objectives

The general objectives of this research program are: a) to conduct an experimental investigation of pulverized coal gasification processes to determine optimum operating conditions. The extent of char burnout, the product distribution and the sulfur and nitrogen pollutant formation levels will be criteria for determining optimum conditions. Variables to be considered will include coal type, pressure, steam/oxygen/coal ratios, coal particle size, gasifier injector configuration including swirl, preheat temperature and secondary/primary mass flow and velocity ratios; b) to obtain detailed gasification maps of gas and particle profile data of composition inside the gasifier for a family of coal types in order to determine important rate processes and to provide basic data for evaluating the predictive code; c) to complete the development of a generalized, two-dimensional model for predicting details of entrained coal gasification, compare the results to laboratory profile measurements and apply the code to a series of industrial gasifiers. Specific tasks that have been outlined for accomplishment during this Phase 3 study are listed below.

Task 1. Pulverized Coal Gasification Measurements

The existing entrained coal gasifier will be used to conduct an investigation of entrained coal gasifcation. Operating parameters such as jet velocities, pressure, gasifier injector configuration including swirl, coal/steam/oxygen ratio, etc. will be varied parametrically in order to identify ways of optimizing coal gasifier reactions and operation. Gasifier "maps" will be obtained for selected coal types and operating conditions. These maps will be used to validate the two-dimensional computer code and to determine rates of mixing, reaction and pollutant formation.

Task 2. Gasifier Model Development

Previous work on the one-dimensional code is complete and the code is now functional (1-4). The two-dimensional code is presently being developed under funding by both this DOE contract and the Phase 3 EPRI contract (EPRI Contract No. RP-364-3). The partially completed, two-dimensional code will be completed by including routines which will model coal devolatilization, char reaction and radiation heat transfer. The completed code will be compared to test results obtained from the cold-flow facility, from previous clean gas (natural gas/air) combustion tests, from coal/air combustion tests and from coal/steam/oxygen gasification tests. Work will be initiated to extend the two-dimensional code to three-dimensional gasifiers.

Task 3. Cold-Flow Mixing Experiments

The cold-flow jet mixing experiments will be conducted to support the model evaluation and the coal gasification test program. Mixing and recirculation rates of both the gas and particulate phases will be investigated with swirl introduced into the secondary jet. Jet mixing tests with pulverized coal dusts in sizes that correspond to actual combustion tests will be made. The fluctuating velocity and turbulent intensity levels of clean gas jets will also be made.

Task 4. Reporting and Application to Industrial Needs

Detailed technical seminars will be given to at least three industrial companies in order to guide the coal gasification research and transfer the research results to industry in as timely a manner as possible. Additionally, the Industrial Advisory Panel will continue to be used to provide technical recommendations, industrial interaction and technical exchange. One meeting of the Industrial Advisory Panel at BYU is planned. Copies of all contract reports and related publications will be forwarded to the Advisory Panel members. Quarterly and final technical reports will be treated and forwarded to the DOE program manager for review and approval prior to publication.

SUMMARY OF PROGRESS DURING QUARTER

Task 1. Pulverized Coal Gasification Measurements

Several tasks were completed during the reporting period. These include the following:

- A new team of graduate and undergraduate students was formed to conduct the tests.
- The additional coal types were identified, ordered and have been received.
- The design of the hardware modifications to introduce swirl into the secondary stream was initiated.
- Minor modifications were made to the gasifier to allow laser diagnostics to be made on an independently funded study with LASL (University of California order number CA4-L49-7338J-1).
- A Master of Science thesis (5) and a PhD dissertation (6) based on the previous Phase 2 study (2) were nearly completed. These documents include extensive data analysis of previous test results.

Task 2. Gasifier Model Development

Two-dimensional model development tasks which were underway or completed include the following:

- A Gaussian PDF was substituted for the top-hat PDF in BURN, and parametric runs were made.
- The Lagrangian particle turbulent dispersion module was completed and predictions made for conditions from the BYU cold flow facility.
- Work on the reacting coal submodel is progressing into the final stages of debug.
- Formulation on the radiation submodel is near completion and coding has been initiated.

These remaining modules are all that are needed for completion of the working Pulverized Coal Gasification and Combustion code (PCGC-2).

Task 3. Cold-Flow Mixing Experiments

Several tasks connected with the cold-flow test program were conducted during the quarter:

- A swirl calibrator device was designed and fabricated to calibrate the actual Swirl Number produced by the moveable-block swirl generator discussed in reference 2.

- The swirl calibrator was installed in the cold flow facility and two tests were conducted at the standard flow rate in the secondary jet to obtain data for calibrating the swirl generator. One additional calibration test was conducted at a reduced flow rate.

- Two other cold flow tests were performed to gather local velocity data under swirling flow conditions. Both tests were conducted under standard flow conditions with the small mixing chamber (206 mm diameter) and without particles. One test was performed with the Swirl Number setting at 0.2 and the second test was performed with the setting at 0.6.

- Other tasks completed include further reduction and analysis of particle size data from the previous series of cold flow coal-dust tests (2), development of a modified procedure for presenting centerline axial decay profiles, and the writing of a Master of Science Thesis (7) covering the cold flow coal-dust tests and the cold flow swirl tests discussed in reference 2.

Task 4. Reporting and Application to Industrial Needs

This report is the first quarterly report on this study. Other reports, theses, and papers as well as several contacts and interaction with industry are summarized in the section entitled Detailed Description of Technical progress.

DETAILED DESCRIPTION OF TECHNICAL PROGRESS

Task 1. Pulverized Coal Gasification Measurements

Technical Approach

An entrained flow gasifier, which has been designed and constructed using funds from the previous Phase 1 (1) and Phase 2 (2) studies, is being used to accomplish the experimental gasification tasks of this study. A schematic of the gasifier is shown in Figure 1. The gasifier, which was designed to operate at pressures of up to 2000 kPa (20 atm) has a primary nozzle diameter of 12.7 mm, and a coal processing capacity of up to 136 kg (300 lb) of coal per hour.

The basic experimental approach used in the reactive tests is to obtain a particle-gas sample from inside the reactor using specially designed water-quenched probes which rapidly terminate chemical reaction and keep ash/slag from adhering to probe walls. Analysis of key chemical tracers (Ar, He) from primary and secondary streams indicate directly the extent of local mixing. Particulate materials in the sample are separated and analyzed to determine the rate of particle mixing and reaction and also to determine the ash, volatile matter, and possibly sulfur and nitrogen content for the reacting cases. Reacting gas samples are analyzed to determine such quantities as CH_4, CO, CO_2, and H_2. This information provides direct measurement of the extent of coal or char gasification, and the extent of sulfur and nitrogen pollutant formation. Detailed information on local chemical composition serves as the basis for interpreting rates of mixing and particle reaction.

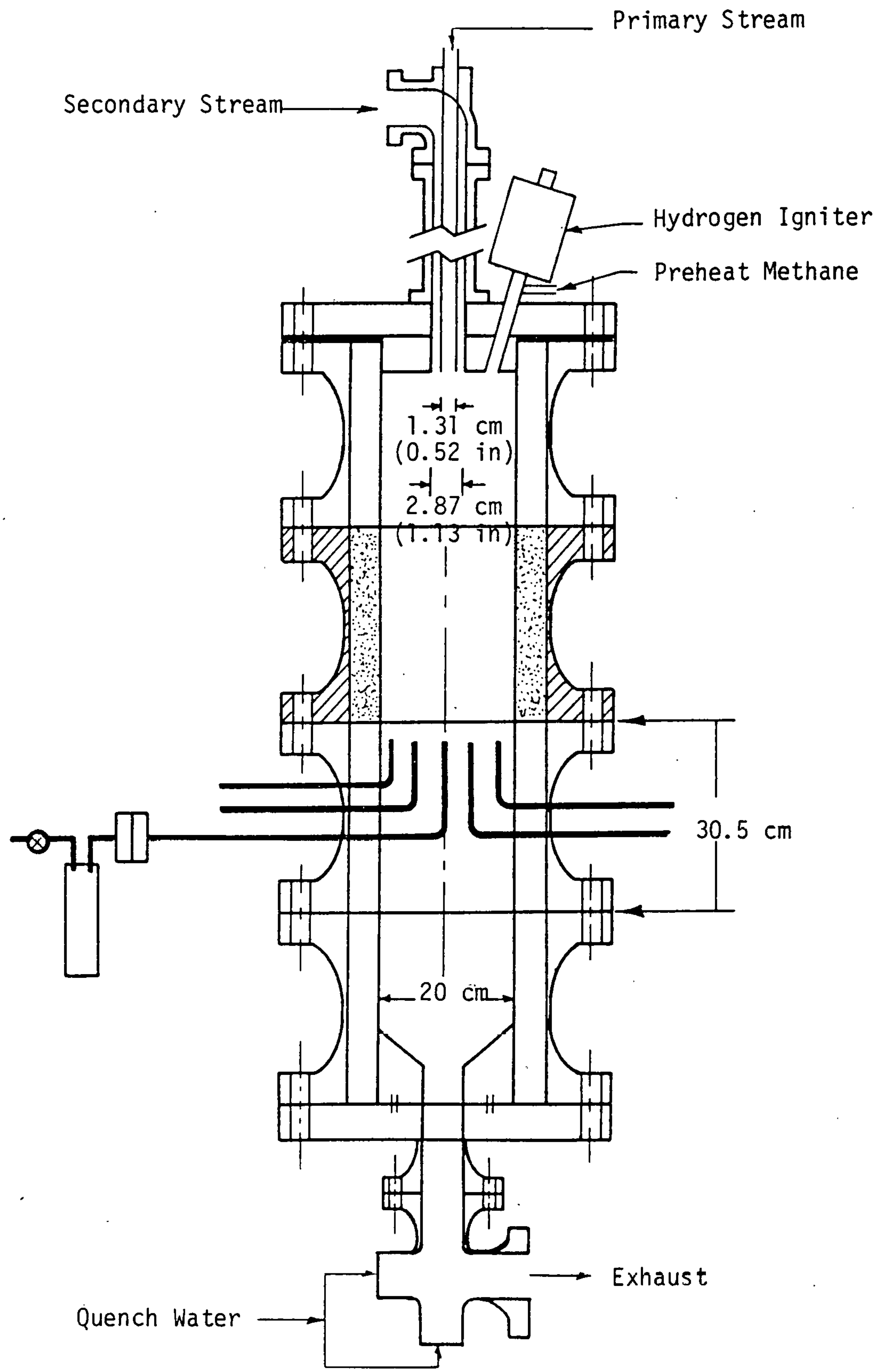


Figure 1. Schematic of high pressure entrained gasifier.

Accomplishments During Quarter

Several tasks were completed during the first quarterly reporting period. A new experimental research team was formed and preparation of the facility for the first optimization tests was begun. The new research team consists of one M. S. student (Guy Lewis) and three undergraduate students (Stephen Kramer, D. Ronald Anderson, and Wesley Pack Jr.).

The design of the hardware modifications necessary to introduce swirl into the secondary stream was initiated. The swirl block design used at Ijmuiden (8), which has been successfully used in the previous cold-flow program (2) and in the related coal combustion program (4), will be used. The swirl blocks will be initially designed to provide a variation in secondary Swirl Number of 0 to 3. This hardware is very versatile and it has been found (4) that with minor modifications, the Swirl Number range can be easily changed.

The additional coal types which will be investigated during this program were identified, ordered and received. A high moisture lignite, a high-nitrogen, high-volatile bituminous coal, and a low-volatile, sub-bituminous coal were selected. Coals were selected that have been studied by others, were in wide use industrially, were easily procurred, and have acceptable characteristics (i.e., grindability, agglomerating characteristics, etc.). Some of the sources contacted for information were MIT, University of Utah, Environmental and Energy Research Corp., Bituminous Coal Research Inc, AMAX Coal Company, Gilberton Coal Company, Consolidation Coal Company, Institute of Gas Technology, North American Coal Company, National Coal Association, Peabody Coal Company, Swisher Coal Company, as well as many mines. Several literature sources were consulted also (Keystone Coal Industry Manual, 1979; IGT, 1976 and Combustion Science and Technology, 1978 an 1979). Three coals from those suggested were selected. These coals met the requirements and their specifications make them very amenable to study. These coals, their source and typical analysis are summarized in Table 1. The coals will be labeled, cataloged, and characterization initiated. This will include pulverization, ultimate analysis, proximate analysis, ash elemental analysis and size distribution measurements. Samples will be submitted to independent agencies for evaluation as well as being evaluated at this facility. Representative samples will then be selected for testing.

The gasifier is also being used to support an independent study sponsored by the Department of Energy with the Los Alamos Scientific Laboratory (LASL). The purpose of this study is to develop laser systems which could be used to make optical spectrographic analyses in pulverized coal gasifiers. The BYU gasifier is being used to provide a realistic gasification environment for the various LASL laser instruments. The gasifier is only being used to provide a test vehicle for a limited number of laser tests. During the quarter, hardware provided by LASL was installed in the gasifier exhaust line. This hardware has a test section which will permit optical access to the gasification exhaust products. These LASL experiments are expected to be concluded during the next quarter but the hardware modifications were so designed that the gasification experiments of this study can be continued without significant interference.

An M. S. thesis (5) and a PhD dissertation based on the experimental results of the previous Phase 2 study (2) were nearly completed during this reporting period. These provide further analysis of the gasification

TABLE 1

SUMMARY OF SELECTED COAL TYPES

Coal	Medium volatile bituminous West Kentucky TRW #1	Sub-bituminous Bel Ayr Mine Gillette, Wyo.	High moisture lignite Knife River Mine Beulah, North Dakota
Source	EER 8001 Irvine Blvd. Santa Ana, Calif.	AMAX Coal Co. 105 S. Meridian Indianapolis, Indiana	Knife River Coal Co. 1915 Kaveney Drive Bismark, North Dakota
Ultimate Analysis (Wgt. %, dry)			
C	70	63	41
H	4.7	4.4	NA
N	1.4	0.9	NA
S	1.0	0.4	1.1
Ash	17.8	8	12
O_2	5.2	15	NA
Moisture (Wgt.%)	6.5	30	34
Volatiles (Wgt. %)	18	43	47

and pollutant formation results of that previous study (2). Some additional findings have resulted from these analyses which are summarized below.

Steam mole fraction calculations. Steam mole fractions were calculated using a procedure based on mass balances which is developed in detail by Skinner (6), and which was discussed in a previous quarterly report (9). The important step was the development of mass balance equations which contain a mixture fraction based on the gas evolved from the coal. An expression was obtained in which the only unknown quantity was the desired steam mole fraction. All other quantities are derived from analyses of the dry gas and particles.

The values of steam mole fraction obtained for the various samples are summarized in Table 2. These numbers, together with the dry gas analyses, were used to calculate the molecular weight of the gas on a wet basis. Both of these quantities were needed to calculate the parameter ϕ_k, as shown below.

Pulverized Coal Gasification Measurements. The results of mapping tests performed in the BYU gasifier during the fall of 1979 (2) have been further analyzed as a part of thesis work. Total mass balances were used to determine if sampling was isokinetic during these tests. The following procedure was employed. It was first assumed that ash in raw coal was inert. Thus, for a given probe in the reactor:

$$F = W_{ak} m_s / t A_p$$

TABLE 2

CALCULATED STEAM MOLE FRACTIONS
FOR TEST SERIES 3

Test No.	Probe location, cm	X_{H_2O}, calc.
110	0.0	0.330
	1.3	0.428
	2.8	0.427
	5.6	0.390
	8.9	0.413
111	0.0	0.407
	1.3	0.327
	2.8	0.391
	8.9	0.346
112	0.0	0.331
	1.3	0.317
	8.9	0.341
114	2.8	0.451
	5.6	0.440
	8.9	0.404

Tabulated ash mass flux values for values for tests 110 through 112 (2) are tabulated in Table 3.

The mass fluxes in Table 3 were used to construct profiles by plotting mass flux versus the square of the radial distance of the probe from the center of the reactor. From such profiles, an area-average flux ($\overline{F}$) was obtained from tests 110 through 112 as follows:

$$\overline{F} = \int_0^{A_r} F \, dA \Big/ \int_0^{A_r} dA \qquad (2)$$

Average ash mass flux values are summarized in Table 4.

With these average flux values calculated, it was possible to compare the total flow of ash calculated from radial sample profiles to the ash input into the reactor from the coal feeder as a part of the coal. A factor, G, was calculated which was a ratio of the mass flux calculated from the known coal feed rate to the mass flux calculated from probe measurements:

$$G = C \, W_{ar} \Big/ \pi \, r_w^2 \, \overline{S} \qquad (3)$$

G factors for tests 110 through 112 (2) are summarized in Table (5).

Table 5 suggests that the mass balance does not close. Ideally, values of G should be 1.00. Apparently, an excessive amount of coal compared to gas was sampled in all mapping tests analyzed (2).

The primary cause of the above imbalance was believed to be excessively high vacuum pressure in the sample lines. There was no way of controlling pressure in the sample line because the lines were connected

TABLE 3

TABULATED ASH MASS FLUXES

Run	Probe No.	Flux (g/cm^2 sec)
110	1	0.026
110	2	0.026
110	3	0.009
110	4	0.007
110	6	0.007
111	1	0.019
111	2	0.020
111	3	0.011
111	6	0.008
112	1	0.011
112	2	0.015
112	3	0.005
112	6	0.029

NOTE: Fluxes for run 114 are not tabulated. Only three probes operated without plugging during this test and graphical integration in this case would produce dubious results.

TABLE 4

AREA-AVERAGED MASS FLUX VALUES FOR ASH

Run	Flux (g/cm^2 sec)
110	0.00792
111	0.00844
112	0.01566

TABLE 5

SUMMARY OF G FACTORS

Test	G Factor
110	0.206
111	0.194
112	0.105

directly to a bank of evacuated steel sample cells. The sampling system is discussed in great detail elsewhere (2). Because of the problem, a revised sampling system has now been developed which permits regulation of the pressure in the sample lines. The revised sampling system is similar to one used successfully by other investigators at this laboratory (10).

Particle mixing and reaction parameter (ϕ_k). The particle mixing parameter, ϕ_k, is defined as the mass fraction of char in a sample volume consisting of char mass, and gas from primary and seconday streams plus gas mass from devolatilizing and reacting coal:

$$\phi_k = m_k/(m_k + m_{gp} + m_{gs} + m_{gk}) \tag{4}$$

Making a mass balance on the particle tracer (ash was used in this case), gives the following expression for ϕ_k:

$$\phi_k = W_{ax}/W_{ak} \tag{5}$$

Where W_{ax} is the mass fraction of ash in the sample volume, and W_{ak} is simply the ash mass fraction in the char. The development of this expression is found in the PhD dissertation by Skinner (6). In order to calculate W_{ax}, the mass of gas (on a water-included basis) which is associated with a given mass of sample particles must be known. Since the sampling rate in the previously reported tests (2) was determined not to be isokinetic, a correction was derived, based on a forced carbon balance, for the particle mass and the moles of gas obtained to that which should have been collected. This procedure as well as the correction factors, are contained in both Skinner (6) and Price (5). The moles of gas obtained were further corrected to include the water mole fraction as calculated above. A gas molecular weight, on a water-included basis was also calculated.

Table 6 summarizes the values of the ϕ_k which were calculated. Figure 2 is a plot of these values of ϕ_k, with respect to the normalized radial position for the three experiments for which sufficient radial data existed. These runs were made at 63.5 and 94 cm. The runs at the other two axial positions studied, 33 and 48.3 cm, did not give complete radial data profiles due to plugging of the centerline and near-centerline sampling probes.

Figure 3 is an axial decay plot of ϕ_k versus the normalized axial position (z/r_1). The core length obtained using this plot is between 23.9 and 31.9 cm, based on 70% confidence limits.

Task 2. Gasifier Model Development

Technical Approach

This activity is directed towards construction of a two-dimensional steady-state, turbulent, coal combustion computer code in axi-symmetric coordinates for predicting detailed local mean properties. This model will be useful for data analysis, sensitivity analysis of physical parameters, scaling, and ultimately for design and analysis of pulverized fuel combustors and gasifiers. As a first step, the description of a diffusion-limited, gas phase combustion model (BURN) was formulated, coded and evaluated. This activity was reported by Smoot et al. (2). A brief outline of the major accomplishments of that contract pertaining to the two-dimensional modeling work includes the following: 1) Formulation, coding, and completion of a two-dimensional, axi-symmetric, turbulent gaseous combustion model. The model includes the effects of turbulent

TABLE 6

CALCULATED VALUES OF THE PARTICLE MIXING AND REACTION PARAMETER (ϕ_k)

Test No.	Probe Location	ϕ_k
110	0.0	0.348
	1.3	0.398
	2.8	0.190
	5.6	0.142
	8.9	0.197
111	0.0	0.381
	1.3	0.290
	2.8	0.230
	8.9	0.149
112	0.0	0.223
	1.3	0.224
	8.9	0.214
113	5.6	0.116
	8.9	0.176
114	2.8	0.273
	5.6	0.099
	8.9	0.153

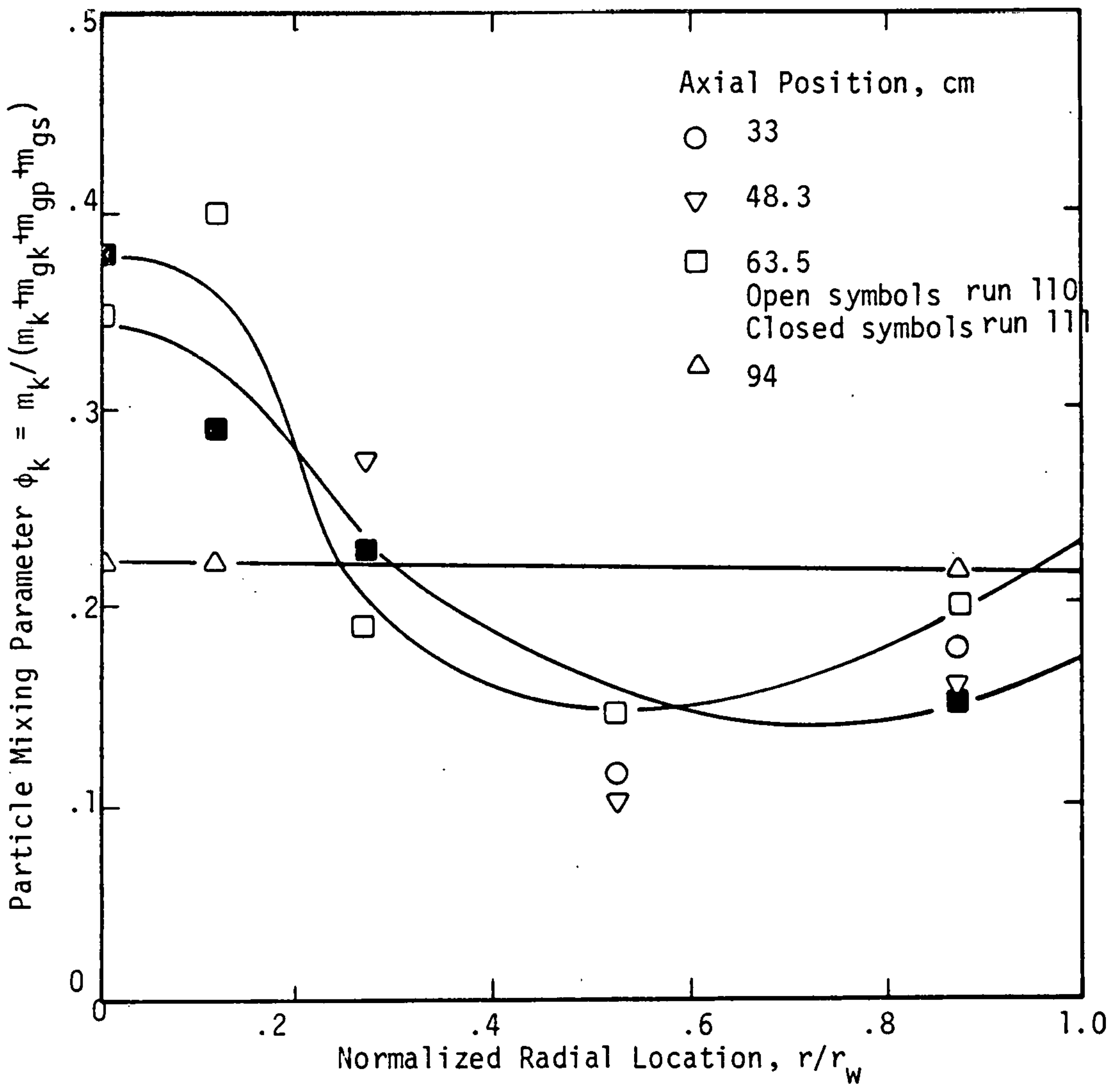


Figure 2. Radial profiles of particle mixing parameter

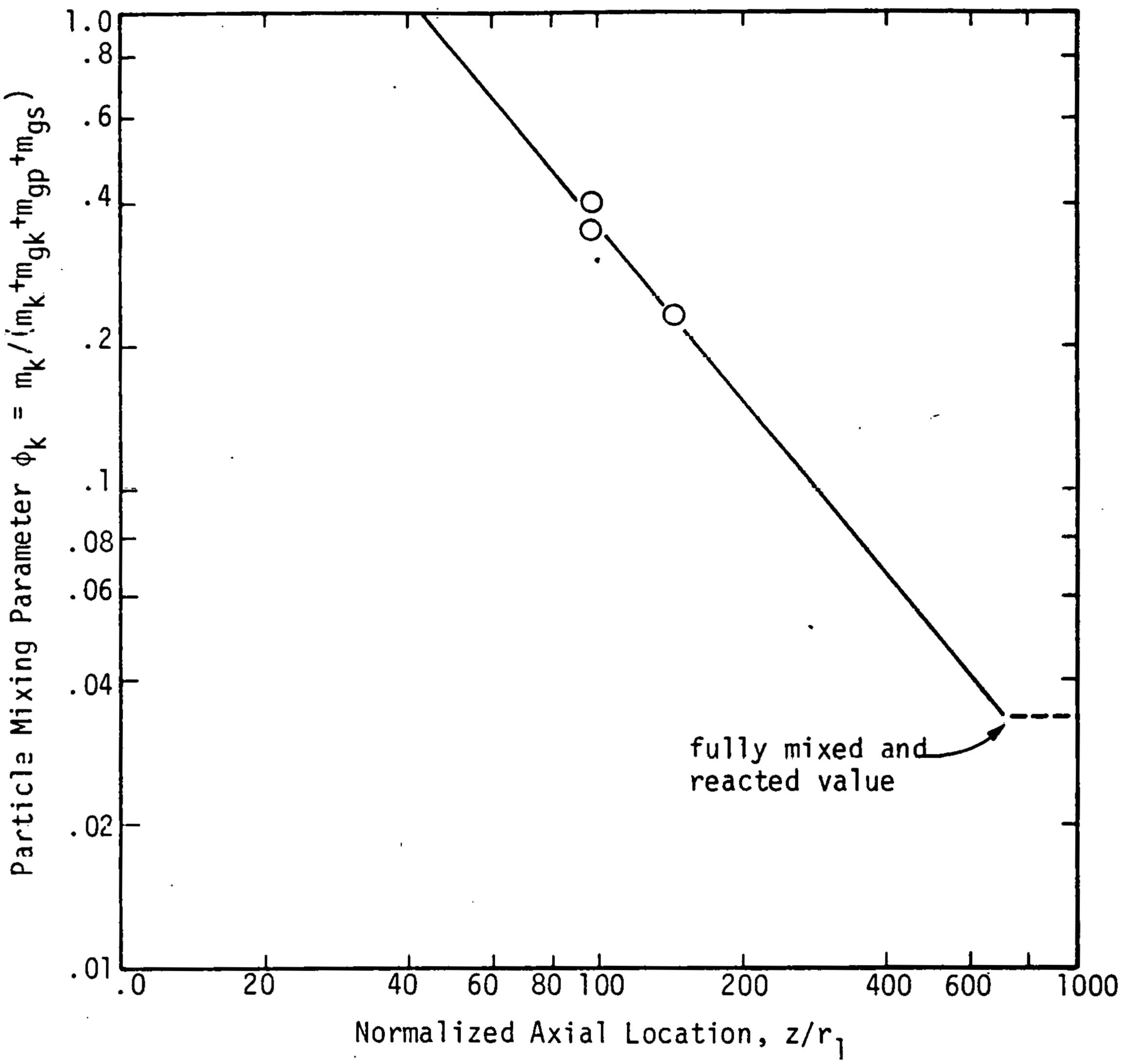


Figure 3. Axial particle mixing parameter profile

fluctuations on the composition and other properties of the reacting flow field by means of a probability density function approach; 2) Application of the gaseous combustion code to several combustion systems including cold flow mixing and reacting combustors; 3) Evaluation of the code by comparison of predictions to measured properties. The experimental data base included measurements at this laboratory as well as other laboratories; 4) Comparison of model predictions with the results of other combustion models being developed at other laboratories. 5) Continuation of the formulation of a technique to include reacting coal particles in the turbulent combustion code. This formulation includes the interactions of the turbulent gas field with the motion of the particles as well as the effect of the turbulent fluctuations on the gas phase chemical field.

At the end of that contract it was recommended that: 1) The probability density function (PDF) approach to combusting systems is a viable method for incorporation of the fluctuations caused by turbulence; however, further investigations and determinations of the shape of the PDF are required; 2) The ability to model turbulent gaseous combustion is far enough advanced to permit incorporation of reacting coal particles. These issues have been addressed during the first quarter of this contract and are discussed next.

Accomplishments During Quarter

PDF. BURN was originally formulated using a top-hat probability density function for predicting average field variables from fluctuating properties. A more naturally-occurring probability density function

(PDF) is the Gaussian distribution. Smith (11) suggested that the Gaussian PDF might be a solution to the lack of agreement between theoretical and experimental concentrations of CO and H_2. The equation for the Gaussian PDF is:

$$P(f)=[1/(2\pi g_f^{1/2}] \exp [-(f-\bar{f})^2/2g_f] \tag{6}$$

where $\bar{f}$ is the average value of the conserved scalar f, and g_f is the variance of f. Intermittency is evaluated using the error function:

$$\alpha_s = [1/(2\pi)^{1/2}] \int_{-\infty}^{u} \exp [-z^2/2] \, dz \tag{7}$$

$$\alpha_p = [1/(2\pi)^{1/2}] \int_{L}^{\infty} \exp [-z^2/2] \, dz \tag{8}$$

where $u = f/g^{1/2}$ and $L = (1-f)/g^{1/2}$

The tabulated values for the error function were numerically fitted with a cubic spline. The Gaussian PDF was used in four parametric predictions and compared with Smith's (11) corresponding top-hat predictions. The maximum temperatures predicted by the Gaussian PDF were at most 10% higher than those predicted using the top-hat distribution, and the composition of O_2 in the gas phase differed somewhat for the two distributions in regions of high fluctuations. The Gaussian distribution also predicted profile curves that were smoother, in general, than those predicted by the top-hat distribution. Overall, the Gaussian distribution seemed to make little difference from top-hat distribution predictions, especially in regions of small fluctuations. This result leads to the conclusion that the precise form of the PDF makes relatively little difference in the model predictions. This result was also suggested by Gosman, et al. (12).

Particle Phase Formulation. This approach is based on the PSI-CELL technique of Crowe et al. (13). The method does not account for particle-particle interactions and thus would not be applicable to highly loaded, particle-gas flow nor to general two-phase flow systems. It is intended to be applied to dispersed flow systems. The model is based on following the trajectories or paths of representative particles through the gas phase field in a Lagrangian fashion. These particles are then treated as sources of mass, momentum and energy to the gaseous phase. Crowe et al. (13) discussed the basic concept, the derivation of the gas flow equations, particle equations and source terms.

Briefly, the particle velocities, trajectories, temperatures and composition are obtained by integrating the equations of motion, energy and component continuity for the particles in the gas flow field. This is done with a Lagrangian approach, while recording the momentum, energy and mass of the particles in crossing cell boundaries. In this straightforward manner, the net difference in the entering and exiting particle properties for any given cell provides the particle source terms for the gas flow equations.

Particle Lagrangian Equations. To evaluate particle properties and to determine the source terms in the gaseous Eulerian equations, the particle Lagrangian equations of motion, energy and continuity are solved.

The Lagrangian equation of motion for a single particle is:

$$\alpha_p \, d\vec{v}_{pc}/dt = \{A_p \rho C_D(\vec{v}_g - \vec{v}_{pc})|\vec{v}_g - \vec{v}_{pc}|/2\} + \alpha_p \vec{g} \quad (9)$$

The first term on the right-hand side of Eq. 9 depicts the aerodynamic drag force, and the last term represents the body forces. Crowe (13, 14) points out how and why this equation neglects virtual mass, Basset force, pressure gradient force, Saffman lift and Magnus forces.

For Reynolds Numbers up to 1000 (based on particle diameter and gas-particle relative velocity) the following correlation for the drag coefficient is suggested (15):

$$C_{DO} = (24/Re)(1 + 0.15\,Re^{0.687}) \quad (10)$$

Particle reaction can reduce the drag coefficient due to mass efflux according to the following suggested relationship (16):

$$C_D = C_{DO}/(1 + B_m) \quad (11)$$

where B_m is the blowing parameter for mass transfer and is discussed in Smith and Smoot (17).

If the gas flow field is assumed constant over the time of integration, Eq. 9 can be integrated once analytically to yield the convection velocity of the particle. In the two-dimensional, axi-symmetric coordinate system, this results in the solution of both components of the velocity vector.

The effect of turbulence in the gas flow field on the particle is a difficult issue. It is assumed that the total particle velocity is composed of a convection velocity and a turbulent diffusion velocity:

$$\vec{v}_p = \vec{v}_{pc} + \vec{v}_{pd} \quad (12)$$

The convection velocity is calculated from Eqs. 9 through 11. The diffusion velocity is approximated by a gradient diffusion law:

$$j_p = \rho_p^b \vec{v}_{pd} \doteq - \Gamma_p \vec{\nabla} \rho_p^b \qquad (13)$$

The particle eddy diffusivity, Γ_p, is related to the gaseous turbulent momentum diffusivity by:

$$\Gamma_p = \mu_e/(\rho_g \sigma_p) \qquad (14)$$

Thus, the turbulent particle diffusion is related to the gas phase turbulence properties through a turbulent particle Schmidt Number, σ_p. This turbulent Schmidt Number is a function of particle size. There is significant uncertainty in its value (14,18). Cold flow data for gas-particle systems being obtained at this laboratory provide a data-base for evaluation of this parameter.

After determining the particle velocity, a straightforward numerical integration of the velocity equation yields the particle position. The particle trajectory is traced by following this process in space and time.

The Lagrangian equation of energy for a single particle is:

$$\frac{d(\alpha_p h_p)}{dt} = Q_{rp} - Q_p - r_p h_{pg} \qquad (15)$$

In this equation, the total enthalpy of the particle is computed from radiation, convection, conduction and reaction. The net radiative heat transfer rate from the particle cloud, the gases and the walls to the particle (Q_{rp}) is the first term on the right-hand side of Eq. 15. The net rate of convective/conductive heat transfer to the particle is represented by Q_p. The last term represents the energy lost from the particle due to particle reaction. The form of each of these terms is discussed by Smith and Smoot (17).

The mass of each particle (α_p) is calculated from the equations of continuity for each constituent. In this coal particle reaction model, the particle is composed of specified amounts of raw coal, char and ash.

$$\alpha_p = \alpha_{cp} + \alpha_{hp} + \alpha_{ap} \tag{16}$$

The ash is nonreactive and thus α_{ap} is constant. The continuity equations for raw coal and char are:

$$d\alpha_{cp}/dt = r_{cp} \tag{17}$$

$$d\alpha_{hp}/dt = r_{hp} \tag{18}$$

where r_{cp} and r_{hp} are the reaction rates of raw coal and char.

In this Lagrangian approach, an arbitrary number of particle types is allowed. This is an important feature, since Field et al. (19), George et al. (20) and others have indicated that approximating a pulverized coal system with a non-dispersed particle size might lead to significant error. The description is such that each particle type may have its own properties such as composition, rate of devolatilization, rate of oxidation, etc.

Source Terms. The sources of momentum, energy and mass in the gas phase Eulerian equations due to the presence of the particles are calculated and stored as each particle trajectory traverses each cell in the computational domain.

As previously discussed, the Lagrangian approach calls for representing the particle flow by a finite number of single particle trajectories. The particle number flow rate represented by the single particle computation along any trajectory is initially obtained from:

$$n_{ij} = m_{po} X_{io} Y_{jo} / \alpha_{pjo} \tag{19}$$

where m_{po} is the initial mass flow rate of all the particles, X_{io} is the mass fraction of particles at the ith initial starting point and Y_{jo} is the initial mass fraction of particles of the jth type. The number flow rate along any given trajectory (n_{ij}) is constant.

The source of mass in the Eulerian gas-phase equations for any cell is the change of mass in all particles that traverse the kth cell:

$$(\Delta m_{pij})_{kcell} = n_{ij} \, [(\alpha_{pij})_{out} - (\alpha_{pij})_{in}]_{kcell} \tag{20}$$

Thus:

$$(VS_{pm})_{kcell} = (\sum_i \sum_j \Delta m_{pij})_{kcell} \tag{21}$$

Similarily, for the momentum source:

$$(V\vec{S}_{pv})_{kcell} = \{\sum_i \sum_j n_{ij} \, [(\vec{v}_{pij}\alpha_{pij})_{out} - (\vec{v}_{pij}\alpha_{pij})_{in}]\}_{kcell} \tag{22}$$

The energy source term is analogous but must be balanced for any particle or particle wall radiation:

$$(VS_{ph})_{kcell} = \{\sum_i \sum_j n_{ij} (\sum_\lambda \alpha_{pij\lambda} h_{pij\lambda} - tQ_{rp})_{out} - (\sum_\lambda \alpha_{pij\lambda} h_{pij\lambda} - tQ_{rp})_{in}]\}_{kcell} \tag{23}$$

Computational Techniques. The Lagrangian particle procedure includes a turbulent diffusion velocity which is calculated from a bulk density gradient (see Eqs. 12-14). This gradient is an Eulerian term that is not immediately available as the Lagrangian path is followed. Methods used at this laboratory for obtaining this gradient by counting particles and smoothing Lagrangian density information have not been acceptable. Since the approach is empirical and since a turbulent diffusivity must be specified, the recommended procedure is to calculate a bulk particle density from the gas phase mixture fraction information. The first approximation is to use the particle number density gradient rather than the bulk particle density in Eq. 13:

$$\vec{j}_j = n_j \alpha_j \vec{v}_{jd} \doteq -\Gamma_j \alpha_j \vec{\nabla} n_j \tag{24}$$

The particle number density, n_j, is a conservative scalar and can thus be calculated from the gas phase mixture fraction:

$$n_j = f n_{jp} + (1-f)\, n_{js} \tag{25}$$

This assumes that the particles follow the gas exactly, which of course is not true; this is only used to model the bulk particle density gradient in the particle turbulent diffusion velocity which, as pointed out, is only approximate. This model permits direct computation of the particle trajectories with a given gas phase solution.

Radiation. There are several existing approaches to radiation modeling in pulverized fuel flames (21). Of these approaches, the flux methods are differential in nature and thus, much more amenable to incorporation into the overall proposed scheme. Varma (14) gives some background to radiation heat transfer in industrial furnaces and also reviews the different available techniques. They also show a formulation of a proposed four-flux model for two-dimensional, axi-symmetric geometry. This is the approach to be used in PCGC-2. Coding has been initiated and will continue through the next quarter.

Progress in PCGC-2. The first step in this quarter towards completion of PCGC-2 was to extend BURN to include non-reacting particles. This includes the submodel proposed in this report for the particle dispersion using the Lagrangian trajectories but without the complexities of particle reaction. The code has been formulated, coded and tested. Comparisons have been made with experimental data gathered at this laboratory with the non-reacting, particle-laden jet-mixing facility. The converged, recirculating trajectories computed for the BYU mixing chamber apparatus are shown in Fig. 4. This computation emphasizes the effect of the Turbulent Schmidt numbers on particle dispersion.

Finally, this laboratory is presently coding the reacting particle submodel into the two-dimensional code. The formulation is complete. The coal submodel has been coded, and is in the final stages of debug. Preliminary indications show that numerical instability is introduced when using the simple Euler's method to integrate the particle reaction equations along a streamline. Presently, predictor-corrector methods are being incorporated for the particle energy and continuity equations.

Task 3. Cold-Flow Mixing Experiments

Technical Approach

During the Phase 1 and Phase 2 studies (1, 2), three series of cold-flow tests were performed which emphasized the effects of secondary injection angle, the effects of expanded angle and increased mixing

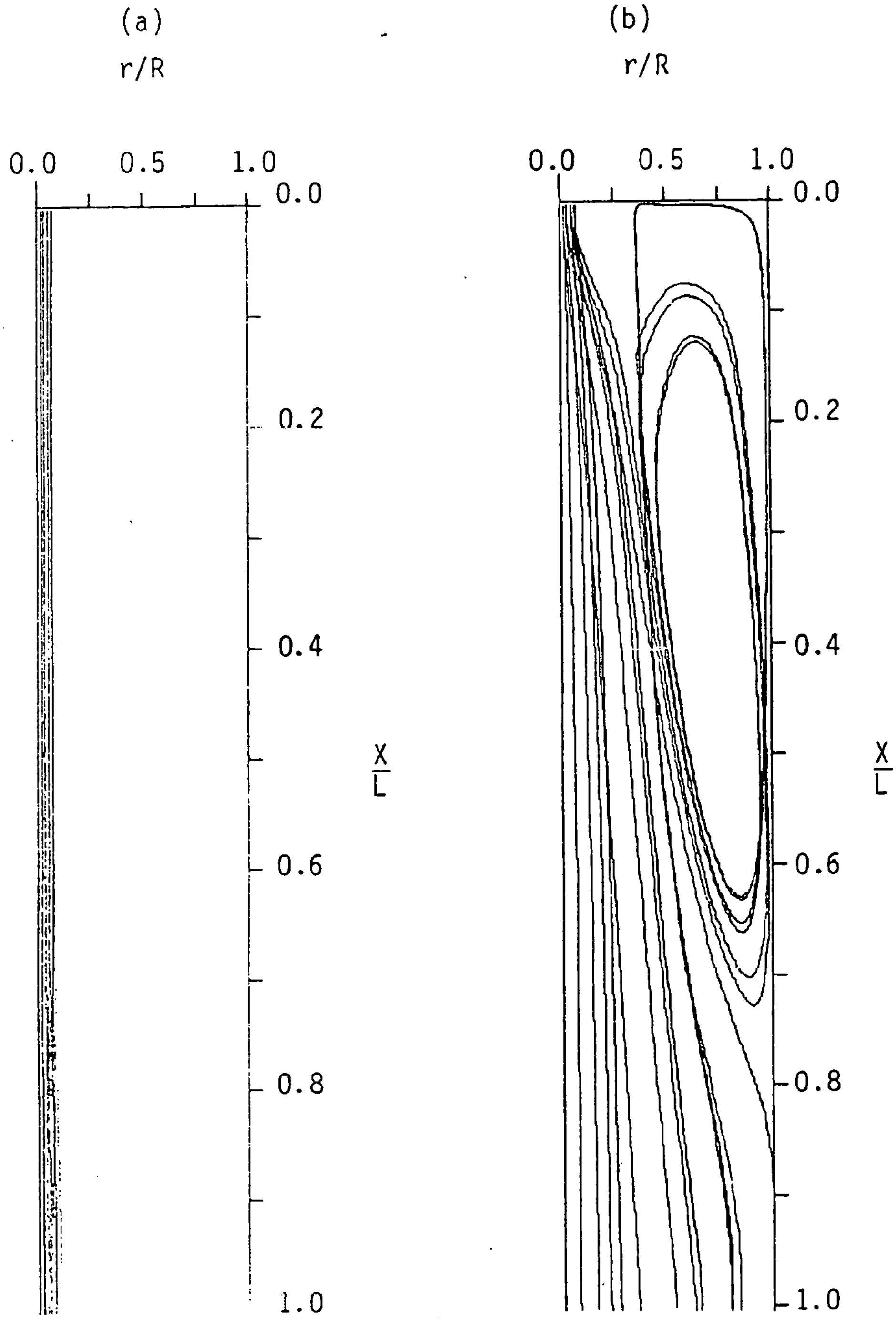


Figure 4. Plot of particle trajectories showing the effect of turbulent particle diffusion. (a) Mean drag only, turbulent diffusion velocity neglected. (b) Mean drag and turbulent diffusion included. Each computation shows 15 trajectories (5 starting locations, 3 particle sizes at each starting location, 20 µm, 50 µm, 100 µm). Turbulent Schmidt Numbers for (b) were $\sigma_1 = 0.3$, $\sigma_2 = 0.4$, $\sigma_3 = 0.8$ for the three particle sizes.

chamber diameter. A fourth set of tests conducted under Phase 2 (2) emphasized the effects of swirl on the mixing process. Swirl, introduced by the addition of a swirl block generator in the secondary stream, was continuously variable from zero up to the maximum design Swirl Number of three. These existing cold-flow hardware components will be utilized in this study to minimize facility construction costs.

Tests are planned to measure the velocity and the turbulent intensity in the jet mixing apparatus with an available hot wire anemometer. This instrument has a capability of measuring very low gas velocities in two dimensions and the turbluence characteristics of the flow. The instrument is relatively fragile and consequently will not be used with coal dust. These velocity data will also be used to quantitatively determine recirculation patterns and recirculation mixing rates for detailed two-dimensional code validation.

Test are planned to obtain cold-flow recirculation and mixing data which can be used as input to the one-dimensional model and which can be used to validate the mixing aspects of the two-dimensional code. The approach and procedures for the jet mixing tests will generally follow that used in previous tests (1-4). In addition to the hot wire anemometer, isokinetic probes will remove samples of gas and particles (in the two-phase tests) at various axial and radial regions in the flow. The extent of gas phase mixing will be determined from the gas sample using argon as a tracer gas. The extent of particle dispersion will be determined from the particle samples. Stagnation pressure measurements using dusty gas probes will also provide velocity data. Probe measurements can be made on the centerline and at other radial positions downstream from the recirculating zones.

<u>Swirl Generator Calibration</u>. The description of the cold flow facility moveable block swirl generator, including hardware and principles of operation, have been discussed in detail (2). One of the favorable characteristics of the Ijmuiden-type moveable-block swirl generator is the ability to easily alter the swirl characteristics of the secondary jet. This is accomplished by adjusting the position of the moveable blocks relative to the stationary blocks with the use of a swirl adjustment rod as illustrated in Fig. 5. The degree of swirl is often characterized by a Swirl Number defined by the equation

$$S = G_\phi / G_x R \qquad (26)$$

where G_ϕ is the flux of angular momentum, G_x is the flux of axial momentum, and R is the exit radius. A theoretical Swirl Number has been derived for the moveable-block swirl generator which calculates S as defined in Eq. 26 as a function of the geometry and position of the blocks. This is based on the assumption of incompressible, inviscid flow. By incorporating the specifications of the swirl generator, it is relatively simple to calculate the theoretical Swirl Number based on block position by determining the relative position of the swirl adjustment rod. This calculated Swirl Number was used to characterize the cold flow swirl tests in the Phase 2 study (2).

The degree of swirl produced by the swirl generator can be obtained directly by measuring the flux of angular momentum and incorporating it directly into Eq. 26. This method was used in the cold flow facility to calibrate the swirl generator. A calibration device was designed and fabricated based on recommendations of Heap (22) to measure G_ϕ directly. A schematic representation of this swirl calibrator is illustrated in

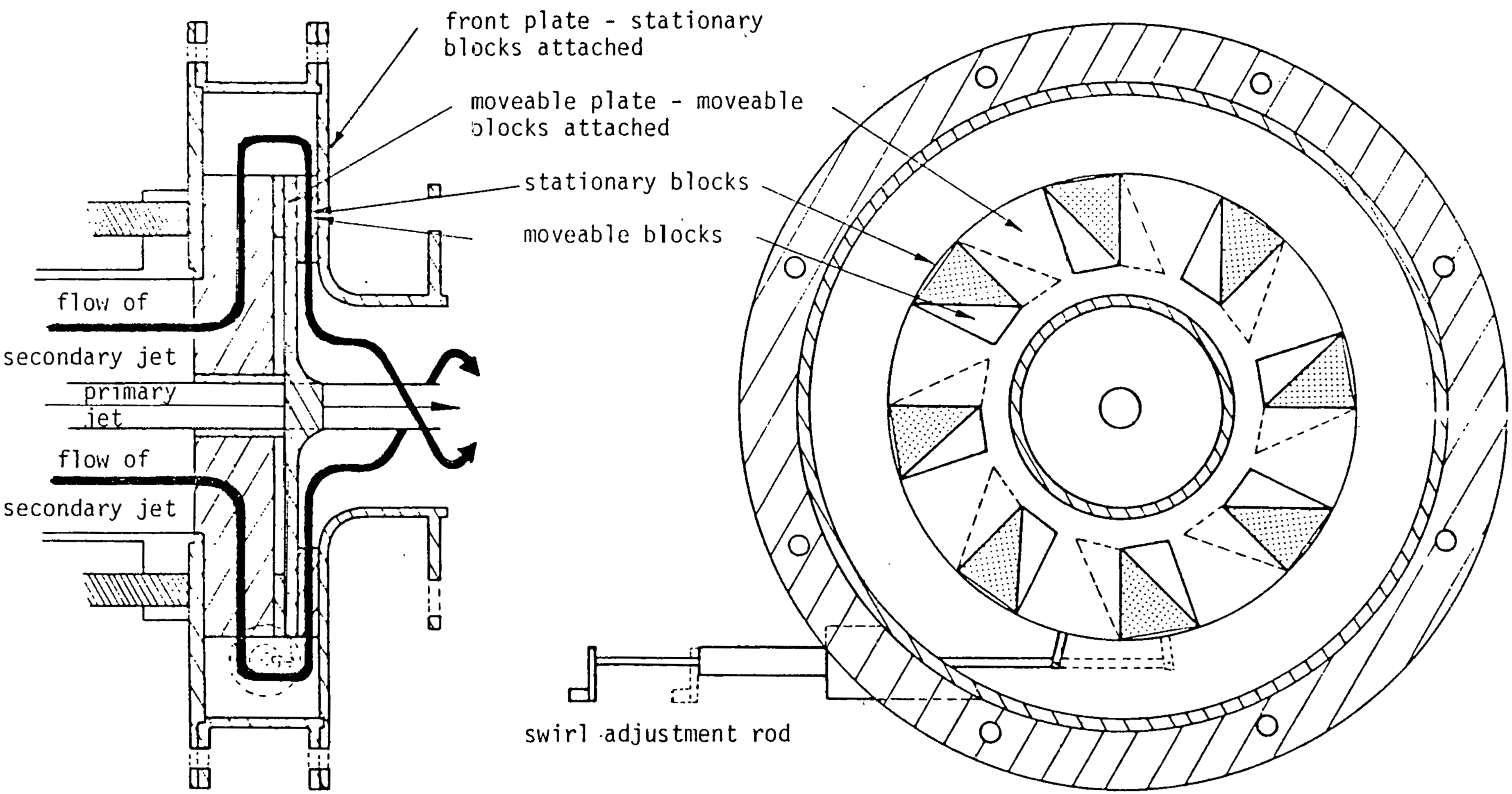


Figure 5. Schematic of cold-flow swirl block generator.

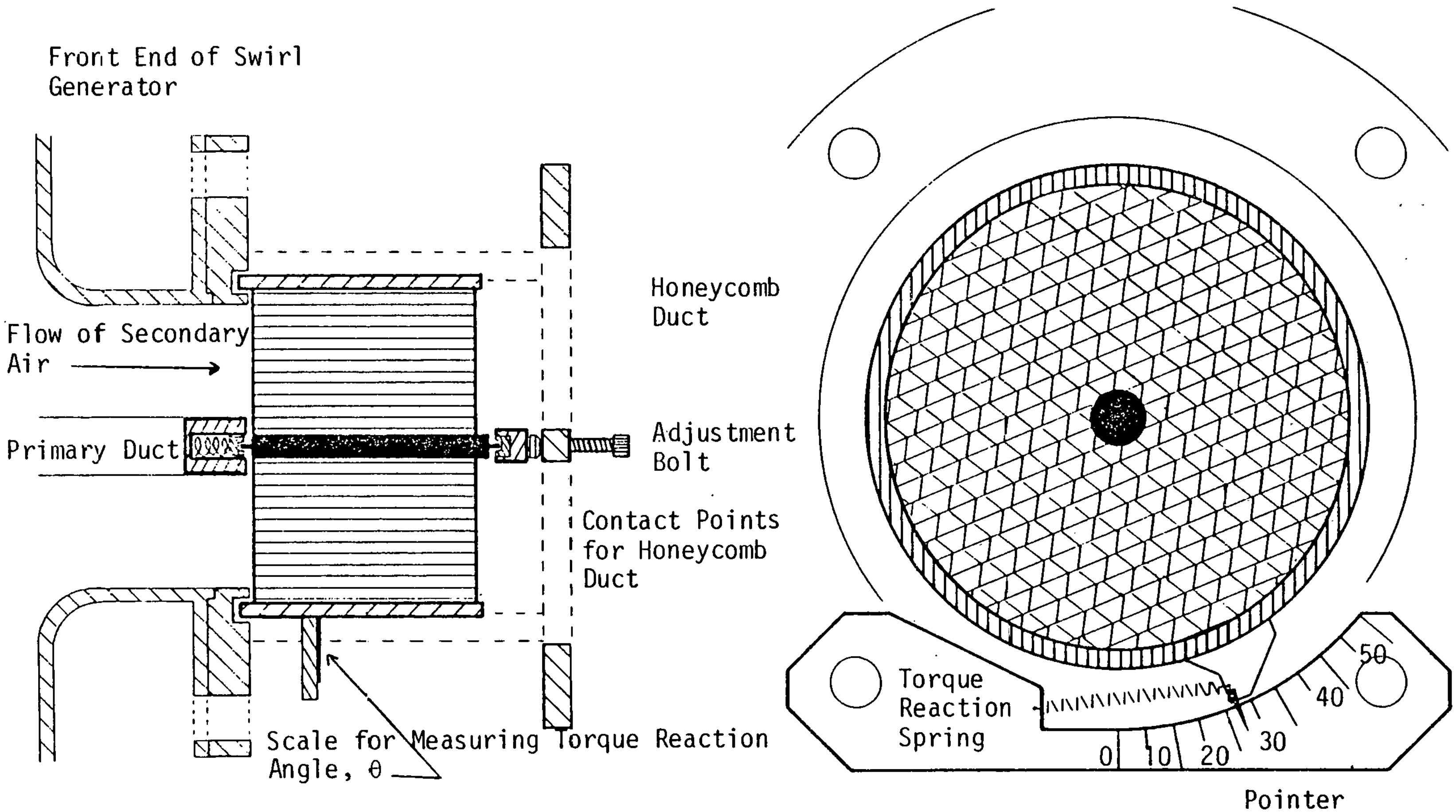
Fig. 6. It consists primarily of a section of honeycomb duct placed directly over the swirl generator exit. The duct is designed to pivot about two axial contact points located centrally on both ends of the honeycomb duct. The duct is precisely balanced and adjusted so that no extraneous forces (i.e. friction, gravity, etc.) can act on it and so that the entire secondary jet is forced to pass through the honeycomb. The individual channels in the honeycomb are approximately triangular and channel length is approximately 20 diameters, where the channel diameter is defined as four times the hydraulic radius. In addition to the two contact points, the honeycomb duct is also attached by a spring to a stationary gauge which measures the reaction torque angle.

When the secondary jet conditions are established and the swirl adjustment rod is moved to the desired position, the swirling secondary jet passes through and exerts a torque on the honeycomb. The duct rotates until the force of the spring on the gauge imparts a torque equal in magnitude to the torque produced by the flow. The angle of rotation can then be measured and the torque calculated by knowing the spring constant and the dimensions of the swirl calibrator. The torque thus measured is G_ϕ where:

$$G_\phi = \int_0^r 2\rho w u \pi r dr \qquad (27)$$

and u is the axial velocity, w is the tangential velocity, and p is the density of the fluid. The linear momentum is determined by:

$$G_x = m^2/pA \qquad (28)$$



a) Side View

b) Axial View (looking upstream)

Figure 6. Schematic views of swirl calibrator for the cold-flow test facility moveable-block swirl generator.

where m is the mass flow rate and A is the area of the secondary exit. The Swirl Number calculated from these measured values is a "secondary" Swirl Number since the flow conditions of the primary jet have not been included.

Three tests were conducted to calibrate the swirl generator. A light-weight and a heavy-weight pre-calibrated spring were used in the tests. Two tests were conducted at standard flow conditions (1965 kg/hr) in the secondary jet using the light and heavy springs. The third test was conducted at reduced flow conditions (1380 kg/hr) using the heavy spring. Measurements were taken at various Swirl Numbers, with care taken to ensure the integrity of the springs and the honeycomb. The results of these tests are illustrated in Fig. 7. It is apparent that the Swirl Number based on the angular position of the blocks underestimates the actual Swirl Number. It is believed that this is due to slight errors in the fabrication of the blocks, as well as the inability to accurately determine the position of the blocks based on the position of the swirl adjustment rod.

Velocity Profile Tests. Two swirl tests were conducted at standard flow conditions to obtain velocity data. Both tests were conducted in the small mixing chamber (206 mm diameter) without particles. One test was conducted at a Swirl Number setting (S) of 0.2 (based on position of the adjustment rod) and the other at a setting of 0.6. Velocity data from previous swirl tests (2) were not obtained due to a leak in the pressure line. Velocity data from the two recent tests are illustrated in Figs. 8 and 9. Both axial and tangential velocities are shown. An effort was also made to correct the velocities for alignment angle

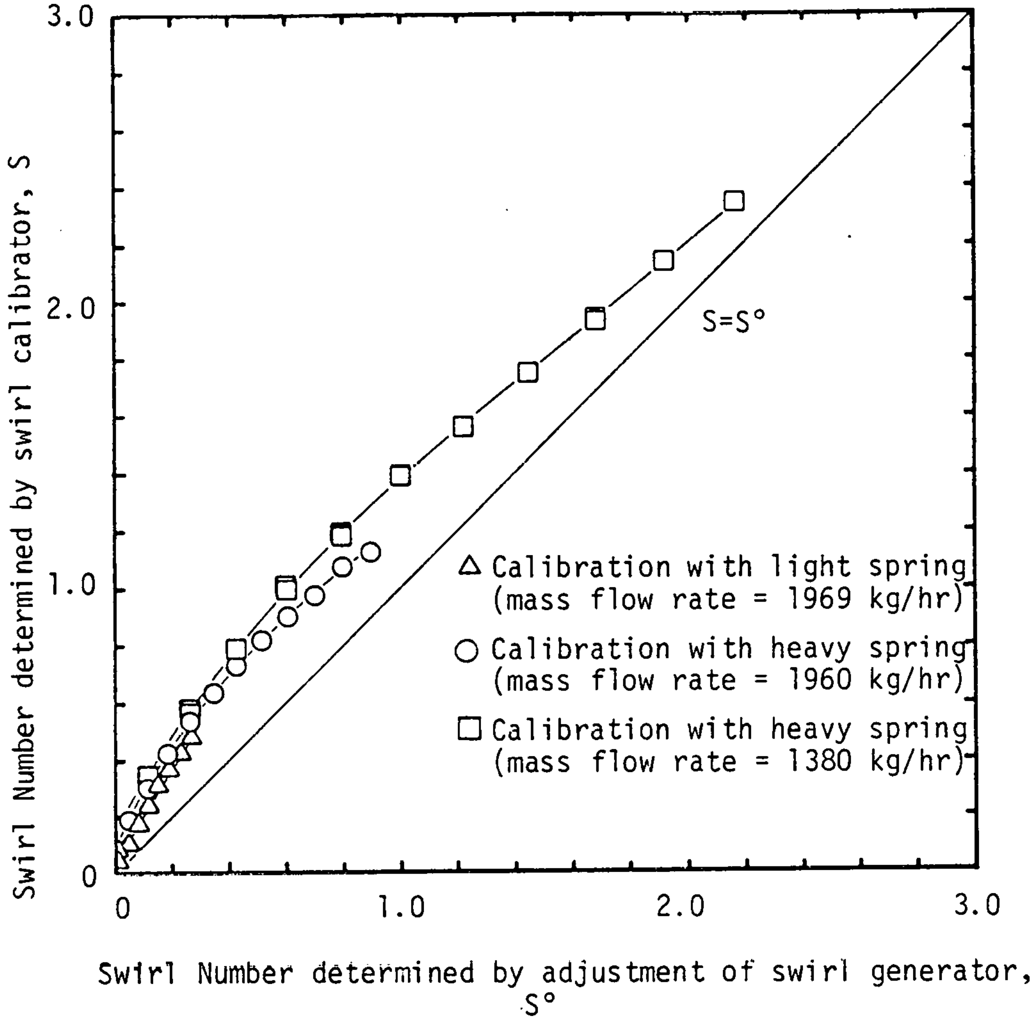


Figure 7. Plot showing Swirl Numbers determined by swirl calibrator vs. Swirl Numbers determined by apparent position of moveable blocks in swirl generator for cold flow test facility.

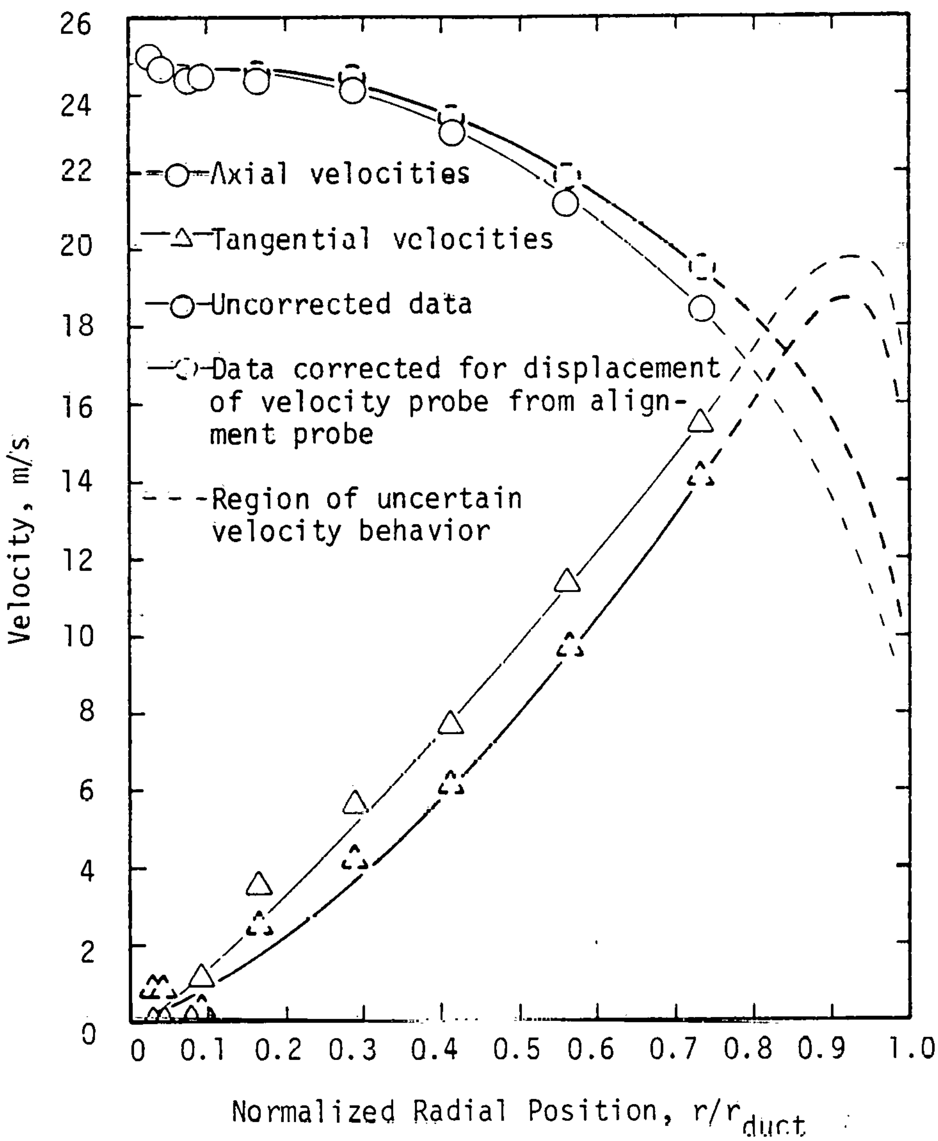


Figure 8. Radial plots of axial and tangential velocities for cold flow swirl test at standard flow conditions with small mixing chamber (206 mm diameter), Swirl Number set at 0.2, axial position of probe at 222 mm from primary exit (z/r_1 = 17.5).

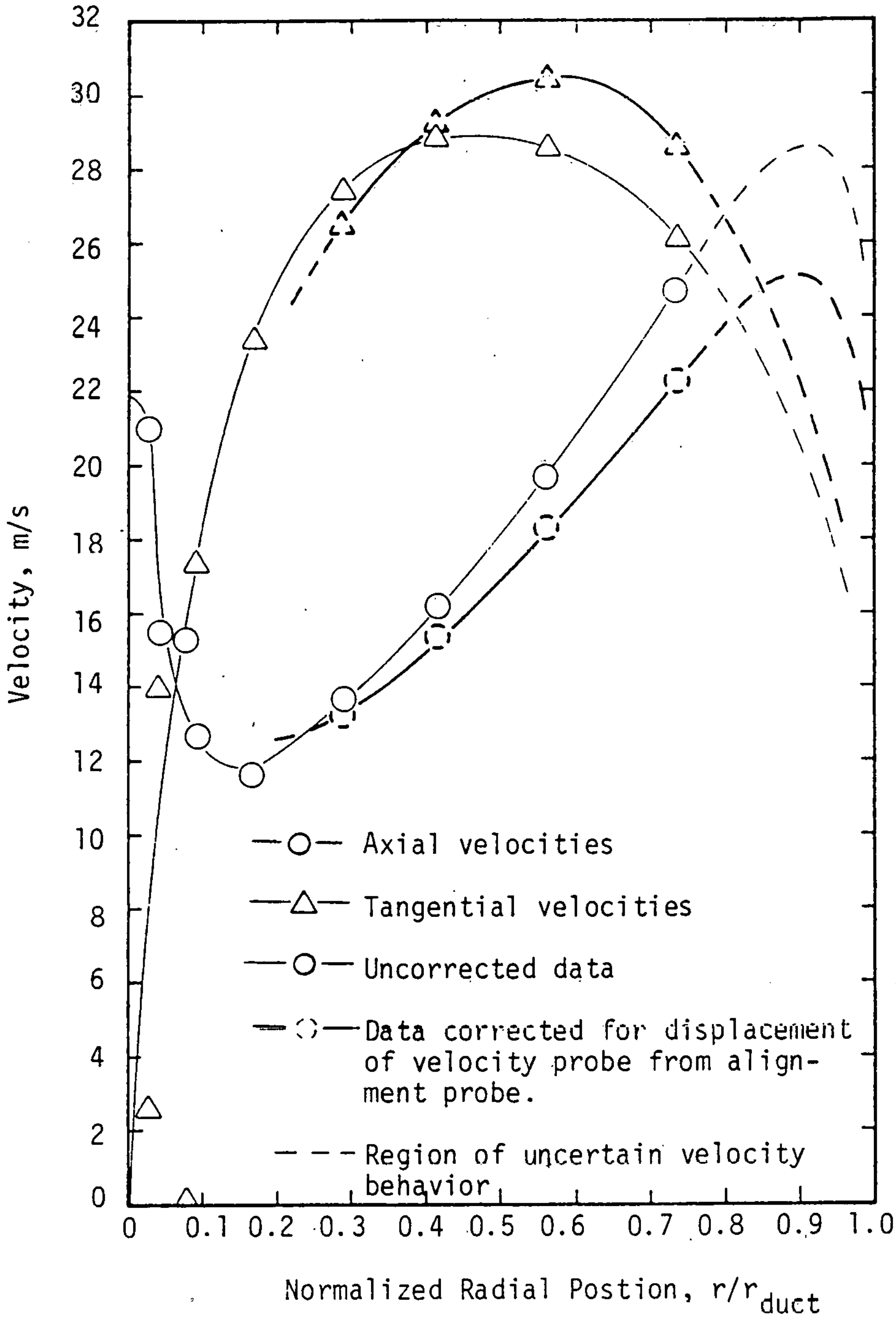


Figure 9. Radial plots of axial and tangential velocities for cold flow swirl test at standard flow conditions with small mixing chamber (206 mm diameter), Swirl Number set at 0.6, axial position of probe at 222 mm from primary exit ($z/r_1 = 1.75$).

error, since the velocity pressure probe is displaced approximately 8 mm in the radial direction from the alignment probes.

The flow regime is altered considerably in going from the lower to the higher Swirl Number. The radial distribution of the axial velocities at S = 0.2 has the appearance of fully developed turbulent pipe flow. Any trace of potential core is gone. The tangential velocity distribution has the appearance of solid-body rotation. At S = 0.6, the axial velocity distribution shows that most of the mass flow is out near the wall. The tangential velocity distribution is also greatly increased over that of the lower Swirl Number. The velocities calculated near the center of the duct for S = 0.6 are somewhat spurious due to the lack of resolution of the probe in this region. Certain anomolies in the data in this region prevented the correction of the velocities. However, it does appear that there exists a potential core in this region which may be caused by the primary jet exiting into a low pressure vortex.

Coal Dust Data Analysis. Particle samples collected during an earlier series of cold flow, coal-dust tests investigating parallel injection and large mixing chamber (343 mm diameter) (2) were recently analyzed on a Coulter Counter. Local mass mean diameter of the particle samples were determined for the respective axial and radial positions in the mixing chamber. Fig. 10 shows radial profiles of the local mass mean particle diameter for several axial positions. The data for each axial station was fitted to a Gaussian type curve using a least squares technique. In each case the larger particles persist toward the center of the duct. Fig. 11 shows the centerline values of the curve fits plotted as a function of axial position. The mass mean diameter of the coal in the primary is also indicated. This figure shows that smaller

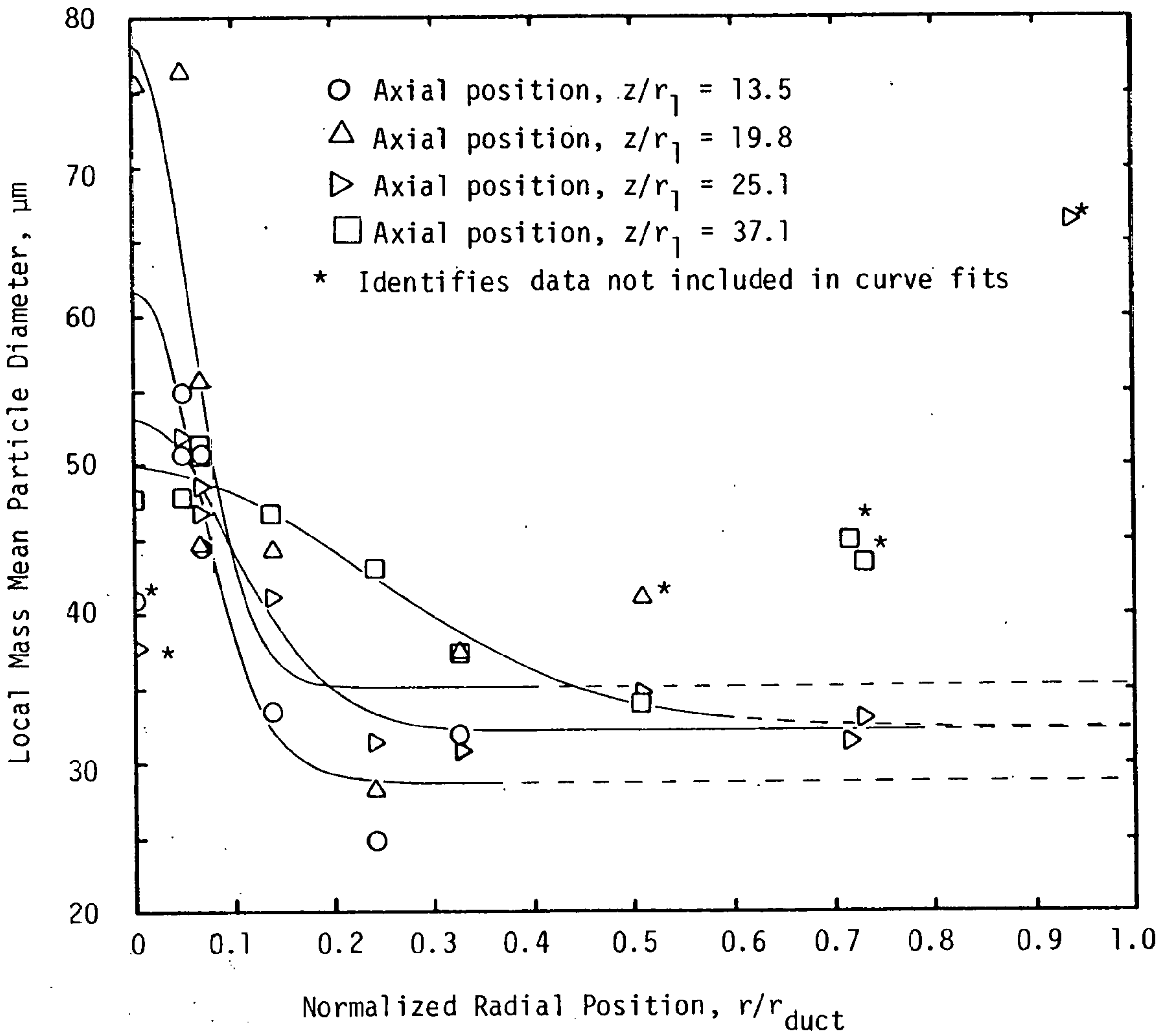
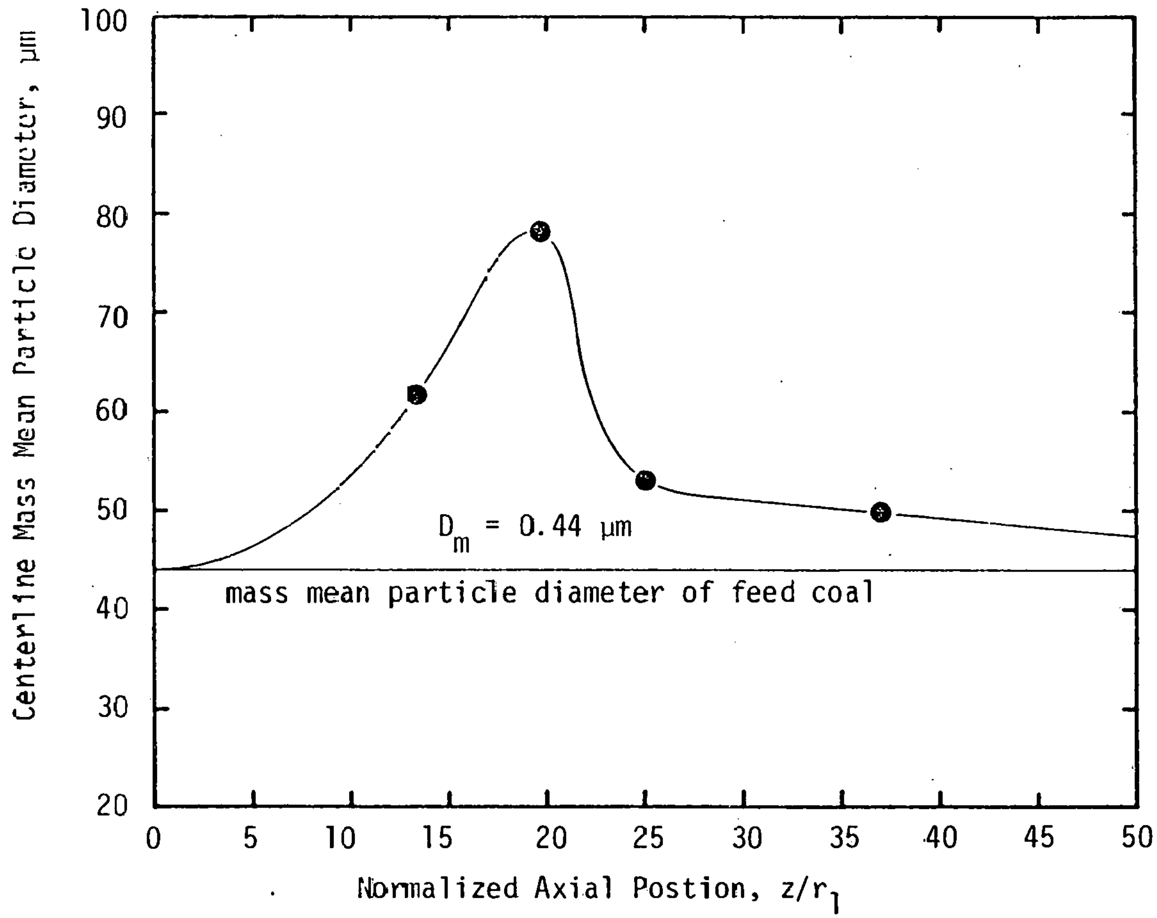


Figure 10. Plots showing effect of radial position on local mass mean particle diameter for cold flow coal dust tests with standard flow conditions, parallel secondary injection, and large diameter (343 mm) mixing chamber.



Fgiure 11. Centerline mass mean particle diameter correlated with axial position for cold-flow coal dust tests with standard flow conditions, parallel secondary injection, and large diameter (343 mm) mixing chamber.

particles disperse more rapidly than the larger ones, causing the mass mean diameter of the particles in the center of the duct to increase as they initially move downstream in the mixing chamber. Then, as continued dispersion takes place farther downstream, the mass mean mean diameter at the center begins to decline back to the primary value.

Modified Centerline Data Presentation. A modified method for presenting centerline axial decay plots was developed during this quarter. Previously, the normalized centerline mixing parameter, ϕ_c for gas and the particles was plotted against a normalized axial position, z/r_1, on log-log coordinates. The data plotted in this manner show a linear relationship and can be analyzed by a least squares linear regression. Although the initial value of the mixing parameter is the same in all cases, i.e. $\phi = 1$ (the value of the primary jet), the ultimate value of the mixing parameter is a function of the composition and flow rates of inlet streams and is therefore not constant. Since greater importance is being placed on the axial location where total mixing finally occurs, it was advantageous to normalize the axial decay plots so that their ultimate, fully-mixed values occur at the same value. This was be achieved by plotting a modified mixing parameter, Φ against log (z/r_1) where Φ is defined by:

$$\Phi = 1 - \frac{\log \phi_c}{\log \phi_m} \qquad (29)$$

where ϕ_m is the ultimate fully mixed value of the mixing parameter. The modified parameter, Φ , varies from 1 at the primary to zero at fully mixed conditions. This device normalizes the conventional axial decay plots and does not alter the axial location of primary core length or fully mixed position as determined by the conventional linear regressions. Fig. 12 illustrates the modified and conventional axial decay plots of gas and particle data for selected test conditions.

In addition to the above tasks, considerable work and progress has also been made in the writing of a Master of Science thesis (7). This thesis, based on these cold-flow test results, will be completed during the next reporting period.

Task 4. Reporting and Application to Industrial Needs

Technical Approach

The six member Industrial Advisory Panel will provide technical recommendations to guide the research and provide industrial interaction and technical exchange. Copies of all publications from the project will be forwarded to the Industrial Panel members. The Industrial Advisory Panel will meet at the BYU laboratory once during the study for extensive review and evaluation of thc program and results. A detailed technical seminar, which documents results of this study, will be presented at selected industrial sites including Babcock and Wilcox, Foster-Wheeler and Combustion Engineering. Three cases will be obtained from entrained gasification projects wherein the one-dimensional and two-dimensional computer codes can be directly applied. The cases will be documented, code solutions obtained and evaluated and applicability of the codes to industrial needs identified. Through the effects outlined above, a very close contact with industrial users of proposed research results will be maintained. At the same time, an effort to find applications for test results will be conducted.

Quarterly and final reports will be prepared and forwarded to both DOE and to the Industrial Advisory committee. Papers, theses and

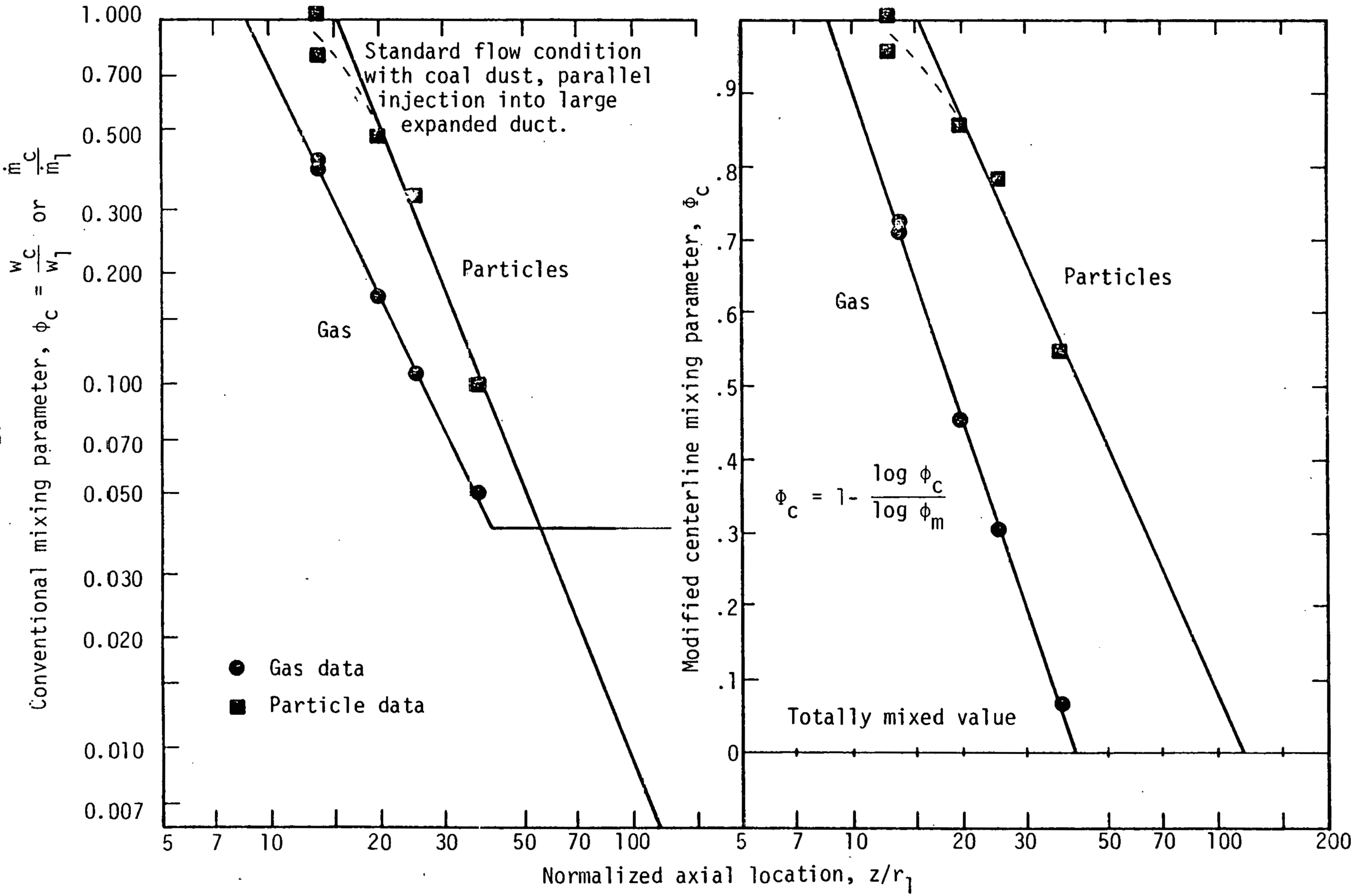


Figure 12. Comparison of centerline axial decay plots of selected test conditions with modified mixing parameter, Φ and conventional mixing parameter, ϕ.

dissertations will be available to the DOE program manager or the Industrial Advisory Committee on request.

Accomplishments During Quarter

The prinicpal investigator presented seminars on coal combustion at Arizona State University (Arizona), Jaycor Corporation (California), Northwestern University (Illinois), Phillips Petroleum Co. (Oklahoma), and Stone and Webster (New York). Work was initiated to implement the one-dimensional code (1-DICOG) at Babcock and Wilcox, Standard Oil Co. of Indiana, and Phillips Petroleum Co. One-dimensional code computations were also completed for Foster Wheeler Corp.

Technical personnel visiting this laboratory during the report period for discussion on coal combustion included, Dr. David Pershing (University of Utah), Dr. Herman Woebcke (Stone and Webster), Dr. Robert Wellek (Department of Energy), Dr. Bernard Blaustein (Pittsburgh Energy Technology Center), Dr. J. Rand Thurgood (Utah Power and Light Co.), Mr. Scott Hassett (Utah Power and Light Co.), Mr. J. F. Farnsworth (Koppers), Dr. David Goracke (Atlantic Research Corp.), Dr. Wen Ho Lee (Los Alamos Scientific Laboratory), and Dr. Gerard de Soete (French Petroleum Institute) Paris, France.

This report is the first quarterly progress report on this study. Other reports and papers on coal gasification or in the related coal combustion work which were completed during the quarter included the technical paper by Smith and Smoot (23), which was accepted for publication in Combustion Science and Technology. A second technical paper, based on the two-dimensional modeling work of Smith and Smoot (24) was submitted to Combustion and Flame for publication. Final preparation on a paper by Smith and Smoot (25) based on the two-dimensional coal code was initiated. Presentations by Skinner and Price, were also accepted for the Fifth Annual Rocky Mountain Fuel Symposium. A doctoral dissertation by Skinner (6) was also nearly completed as were Master's theses by Leavitt (7) and Price (5).

NOMENCLATURE

Symbol	Units	Definition
A	m^2	Area
A_r	m^2	Reactor cross-sectional area
A_p	m^2	Probe tip cross-sectional area
B	---	Blowing parameter
C	$g\ s^{-1}$	Coal feed rate
C_D	---	Drag coefficient
D	m	Diameter
F	g/m^2-s	Ash flux
$\bar{F}$	---	Area-average flux
f	---	Mixture fraction
G		Ratio feed mass flux to probe mass flux, momentum flux
g	$m\ s^{-2}$	Gravitational acceleration
g	---	Mean square fluctuation
h	$J\ kg^{-1}$	Enthalpy
J	---	Total number of particle classifications
j	$kg\ m^{-2}\ s^{-1}$	Mass flux
k	$m^2\ s^{-2}$	Kinetic energy of turbulence
M	$kg\ kmol^{-1}$	Molecular weight
m	---	Mass fraction of species, mass, mass flow rate
m_s		Sample mass
n	s^{-3}	Number flow rate
P	---	Probability density function
P	$M\ m^{-2}$	Pressure
Q	$J\ s^{-1}$	Heat transfer rate
R	m	Exit radius
Re	---	Reynolds Number

r	m	Raidal direction
r	kg s^{-1}	Reaction rate
r_c	m	Total inner reactor radius
S	variable	Source term
T	K	Temperature
t	s	Time
u	m s^{-1}	x - velocity component
V	m^3	Volume
v	m s^{-1}	Velocity, y - velocity component
w_{ak}		Mass fraction of ash in reacted coal particles
w_{ar}		Mass fraction of ash in raw coal
w_{ax}		Mass fraction of ash in sample volume
w	m s^{-1}	z - velocity component
X	---	Mole fraction
x	m	Coordinate
y	m	Coordinate
z	m	Coordinate
α	---	Intermittency factor
α	kg	Particle mass
Γ	variable	Exchange coefficient
Δ	---	Incremental change
ε	m^2 s^{-3}	Dissipation rate of turbulence energy
μ	kg m^{-1} s^{-1}	Dynamic viscosity
ρ	kg m^{-3}	Density
σ	---	Schmidt or Prandtl Number (turbulent)

Subscripts

e	Effective
g	Gas
h	Char
i	Gas species, trajectory starting location, input gas
j	Particle size classification
k	Kinetic energy, cell number, gas species, particle
m	Mass
o	Initial
p	Primary stream, particle
r	Radiation
s	Secondary stream
ϕ	Angular

Superscripts

$\rightarrow$	Vector
-	Reynolds mean
'	Fluctuating component
b	Bulk density

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