***Entrained-flow gasification at
elevated pressure: Volume 1: Final
technical report, March 1,
1985-April 30, 1987***

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Entrained-Flow Gasification at Elevated Pressure

Final Report, Volume I

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Work Performed Under Contract No.: DE-AC21-85MC22059

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Office of Fossil Energy
Morgantown Energy Technology Center
P.O. Box 880
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FOREWORD

This report (Volume 1) summarizes final technical accomplishments made during the twenty-six month study conducted for the Morgantown Energy Technology Center (METC) of the United States Department of Energy (DOE) under Contract No. DE-AC21-85MC22059. Two additional volumes of this final report include a revised user's manual (Volume 2) for a revised two-dimensional code (87-PCGC-2), and the revised "Data Book" (Volume 3) which includes the several sets of data that have been used to evaluate the two-dimensional code. The work period was from March 1, 1985 to April 30, 1987. Work was accomplished under the direction of Dr. L. Douglas Smoot, project director, Dr. Paul O. Hedman, principal investigator, and Drs. Angus U. Blackham and Philip J. Smith, senior investigators. Mr. Gary Friggens was the DOE technical project officer until the summer of 1986 when Mr. Leland E. Paulson became the technical project officer for DOE.

Graduate and undergraduate students who have contributed to the progress reported herein include Larry Baxter, Kevin Boyack, Blaine Brown, Bret Butler, Knute Christensen, Richard Cope, Jeffrey Lindsay, Kenneth Nichols, Mary Rasband, Michael Smith, and William Sowa. Michael R. King, Lynda Richmond, Marlyn Kyle, Shane Olsen, and Linda Ward have provided technician, typing, and drafting services. The National Science Foundation is also acknowledged for supporting a research assistant through a Graduate Fellowship.

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EXECUTIVE SUMMARY

Objectives

The general purpose of this research program was to develop a basic understanding of the physical and chemical processes in entrained coal gasification and to use the results to improve and evaluate an entrained gasification computer model. The first task included the collection and analysis of in-situ gasifier data at elevated pressures with three coal types (North Dakota lignite, Wyoming subbituminous and Illinois bituminous), the design, construction, and testing of new coal/oxygen/steam injectors with a fourth coal type (Utah bituminous), the collection of supporting turbulent fluid dynamic (LDV) data from cold-flow studies, and the investigation of the feasibility of using laser-based (CARS) diagnostic instruments to make measurements in coal flames. The second task included improvements to the two-dimensional gasifier submodels, tabulation and evaluation of new coal devolatilization and char oxidation data for predictions, fundamental studies of turbulent particle dispersion, the development of improved numerical methods, and validation of the comprehensive model through comparison of predictions with experimental results. The third task was to transfer technical advances to industry and to METC through technical seminars, production of a detailed data book, code placement, and publication of results. Research results for these three tasks are summarized briefly here and presented in detail in the body of the report and in supporting references.

Task 1 - Entrained Coal Gasification Measurements

Elevated Pressure Tests. Both parametric variation tests and mapping tests (local measurements made at various radial and axial locations from within the reactor) were completed at elevated pressure with a North Dakota lignite, a Wyoming subbituminous coal, and an Illinois No. 6 bituminous coal. Effects of oxygen/coal ratio, steam/coal ratio, coal feed rate, and operating pressure on carbon conversion and product species concentration were investigated. In-situ data at elevated pressure were obtained for comparison to PCGC-2 predictions and to determine local gas and solids composition, including sulfur and nitrogen pollutant species.

Eighteen parametric variation tests were performed with the North Dakota lignite at pressures from 4.9 to 9.9 atm. Three mapping tests (14 local samples) were performed with the North Dakota lignite at 5.5 atm and three additional mapping tests (9 local samples) were performed at 10 atm pressure. Thirty parametric variation tests were performed with the Wyoming subbituminous coal at pressures from 4.9 to 9.9 atm. Four mapping tests (19 local samples) were performed with the Wyoming subbituminous coal at 5.5 atm pressure, and four mapping tests (19 local samples) were performed at 10 atm pressure. Ten parametric variation tests were performed with the Illinois No. 6 bituminous coal at pressures from 5.3 to 10.1 atm. Four mapping tests (18 local samples) were performed with the Illinois No. 6 bituminous coal at 5.5 atm pressure, and a coal feed rate of about 35 kg/hr and three mapping tests (17 local samples) were performed at 5.5 atm pressure at a coal feed rate of about 50 kg/hr.

Carbon conversion was found to increase with oxygen/coal ratio as expected. In general, the North Dakota lignite had the highest carbon conversion, followed by the Wyoming, and then the Illinois coal. Similar coal rank effects were previously observed by Brown (1985) at atmospheric pressure, and are attributed to the increase of inherent oxygen in the coal, and to the increase in char reactivity as rank decreases. Carbon conversion generally increased with operating pressure for the three coal types when premixing oxygen and coal. Measurements of gas composition and cold gas efficiency are also reported.

The mapping tests at elevated pressure showed a zone of intense reaction near the injector surrounded by a recirculation zone. A zone of slow carbon conversion existed in the lower 2/3 of the reactor. Marked differences in carbon conversion were observed in the elevated pressure maps for the three coals tested. The carbon conversion of the North Dakota lignite was essentially complete by the 22 cm position, while significant reaction occurred between 22 and 83 cm for the Wyoming subbituminous and Utah bituminous coals.

Gasifier Injector Tests. The entrained gasifier computer model (PCGC-2) was used to design and evaluate four gasifier injectors for various oxygen/coal and steam/coal ratios and reactor pressures. The injectors evaluated included a premixed reactants injector (Injector A), a parallel stream, diffusion flame injector (Injector B), a swirled primary stream diffusion flame injector (Injector C), and an impinging secondary stream diffusion flame injector (Injector D). One hundred twenty parametric variation tests and nine mapping tests were completed at elevated pressure with a Utah bituminous coal with these injectors. Effects of oxygen/coal ratio, steam/coal ratio, and operating pressure on carbon conversion and product species concentrations were investigated. Profile data from mapping tests were obtained at elevated pressure for the injectors B, C, and D. Forty-four parametric variation checkout tests were performed with Injector A at pressures from 1.1 to 5.5 atm. Thirty parametric variation tests at pressures from 1.1 to 5.8 atm and four mapping tests at 5.5 atm pressure were performed with Injector B. Twenty-five parametric variation tests were performed at pressures from 1.1 to 5.6 atm with Injector C. One mapping test with Injector C was performed at 5.4 atm pressure, but overheating of the primary injector precluded further testing of this injector type at elevated pressure. An additional four mapping tests were performed at 1.2 atm pressure. Twenty-one parametric variation tests were performed with Injector D at pressures from 1.1 to 5.8 atm. Four mapping tests were performed with Injector D at 5.4 atm.

Injector configuration had a significant effect on the performance of the gasifier, including a strong influence on the conversion of carbon and nitrogen and on cold gas efficiency, product gas composition, and exit gas temperature. In general, Injector C produced the highest carbon conversion and cold gas efficiency, although the details of the effects of the different injectors depended in a complicated way on the flow conditions (Sowa, 1987). Percent nitrogen conversion exceeded percent coal burnout as has been observed in previous gasification tests, and did not depend on injector type.

In both the elevated pressure tests and the injector tests the dominant sulfur species was H_2S for all four coal types at pressures from about 1-10

atm. The amount of H_2S was proportional to the amount of sulfur in the parent coal. Percent nitrogen conversion exceeded percent carbon conversion in all cases. Essentially no exit NO was detected in the high pressure cases except for the Utah bituminous coal with Injector D, which yielded about 100 ppm NO . The exit NO concentrations for the atmospheric tests reached up to 300 ppm, in general agreement with previous studies.

Cold Flow Measurements. A modified laser system was used to obtain specific data on mean axial and tangential and root-mean-square (rms) in a cold-flow facility that was operated at conditions which simulated the flows in the entrained flow gasifier. The study was designed to provide fundamental information about the behavior of flow in such a gasifier and to provide data for the validation of numerical fluid mechanics models. Swirling and nonswirling flows were examined.

Measurements of mean and rms axial and tangential velocities were made in 20 cold-flow cases. Unsteady flow regimes were found. Flow transitions (oscillations between metastable states) were observed and associated with the low Reynolds numbers. Examination of time-averaged results showed that even weak swirl significantly increased the axial velocity decay in the reactor. Comparison of experimental data with PCGC-2 predictions showed that centerline axial velocity was underpredicted near the inlet and overpredicted near the outlet. Predictions generally were insensitive to the details of the inlet profiles.

Spectrographic Measurements. The feasibility of performing non-intrusive gasifier measurements of temperature and species concentrations with a coherent anti-Stokes Raman spectroscopy (CARS) instrument was investigated. A separate DOE instrumentation grant (Grant No. DE-FG05-84ER75153) was received by the laboratory to procure this instrument. The instrument was assembled and demonstrated in a premixed laminar CO/air flame at pressures up to 9.7 atm, and plans were made for its application to a laminar coal flame.

Task 2 - Two-Dimensional Coal Gasifier Model Development

Variable Particle Heat Capacity. The effects of temperature-dependent heat capacity on predicted particle temperature were investigated. Single particle predictions for a constant heat capacity and variable heat capacity particle were performed. The variable heat capacity correlation was adopted from Merrick (1983). Particle temperatures were lower by as much as 500 K, when variable heat capacity was used. The most significant differences occurred during devolatilization. This variable particle heat capacity correlation was added to PCGC-2 as an option. This task was performed with joint funding.

Devolatilization. One- and two-step devolatilization models were investigated. The parameters of the one-step model were found to be dependent on heating rate and/or ultimate temperature. Detailed flowfield predictions were made with PCGC-2 for the data of Kobayashi et al. (1977). Optimized coefficients for the two-step model were found to correlate these data within experimental error over all heating rates. These coefficients were substantially different from those previously suggested. Coefficients for both one- and two-step devolatilization models were tabulated for many coal types.

Char Oxidation. An improved, non-linear, statistical treatment of the Arrhenius-type char oxidation method for data correlation was developed in order to eliminate the inherent errors associated with linearized methods. This has permitted better fits of the oxidation data within the temperature range of the data, and improved rate values when the data are used to extrapolate to higher reaction temperatures. Several sets of char reactivity data important to gasification predictions were used to illustrate the improvements. The char oxidation data tabulated by Field, et al. (1967) were also reanalyzed and successfully correlated with the non-linear method, and limitations of the linear method were clearly illustrated. Coefficients for char oxidation and gasification for a range of coal types were also tabulated for use in PCGC-2.

Turbulent Particle Dispersion. Turbulent particle dispersion was also investigated during this study. The current submodel was critically reviewed and several weak assumptions were identified. A more fundamental model was developed and predictions were compared with results from other models. The new model results agreed with available analytical solutions in all cases where it was tested. It was also slightly more accurate and reduced computer time by approximately three orders of magnitude more than the next most advanced alternative models. The incorporation of this new model as a submodel in PCGC-2 involves rewriting the entire particle portion of PCGC-2, and is being conducted under separate funding.

Numerical Solution Efficiency. This study was focused on the fluid dynamics submodel, where most of the numerical inefficiencies are exhibited in PCGC-2. A simplified version of PCGC-2, called MAXIGAS, was generated for these investigations. Four different approaches were investigated to improve the numerical efficiency or reduce the numerical stiffness (the numerical phenomena that requires large amounts of calculation to resolve small changes in the solution) of PCGC-2: 1) under-relaxation factors, 2) adaptive grid techniques, 3) multigrid techniques, and 4) new techniques to couple momentum and continuity equations.

Several methods of under-relaxation (a reduction in the amount that a variable can change between two iterations) including inertial under-relaxation, were incorporated and evaluated. Best results were obtained using the existing method with adjustments made to the under-relaxation factors based on convergence. This improved the numerical efficiency by about 5-10%. An adaptive grid algorithm was fully coded and evaluated. It was decided that this method did not fully address some of the issues associated with numerical stiffness. A multigrid code was written, and several components evaluated. In conjunction with multigriding, a new continuity-momentum equation coupling technique was also coded.

Model Evaluation. The objective of this subtask was to evaluate PCGC-2 by comparison with measurements and to identify trends and patterns emerging during data prediction and comparison. Joint funding for this effort from this contract and a separate consortium contract (No. DE-F822-85PC-80752) provided for evaluation of non-reacting gaseous and particle-laden flows as well as the gaseous and coal combustion flows.

A previously published Data Book (Smoot and Christensen, 1987) provided a single reference containing detailed experimental data for use in model

evaluation. Nineteen of the 35 cases contained in the Data Book were previously modeled with PCGC-2. The work of this subtask included computations for the remaining 16 cases. The Data Book was also reviewed for errors and corrections were made.

The sixteen cases modeled for this subtask included two gaseous cold flow cases, six particle-laden cold flow cases, five gaseous combustion cases, and two coal combustion cases. Theoretically, coal gasification processes are basically those of fuel-rich coal combustion. The evaluation of simpler flows are essential to understanding the components of the gasification process. Important trends revealed in this study show that PCGC-2 tends to overpredict mixing in non-swirling flows and underpredict mixing in swirling flows. The importance of the correct specification of the inlet velocity profile and inlet turbulence intensity was demonstrated.

Sixty-nine gasification simulations were also performed with PCGC-2. These computations focused on the effects of injector design on gasification and NO_x formation and the effects of feedrate and pressure on NO_x formation. Generally, good qualitative agreement is exhibited in profile comparisons of model predictions and experimental data for CO , CO_2 , and H_2 concentrations. It was observed in predictions with higher-volatile coals that discrepancies existed near the reactor inlet.

Task 3 - Application to Industrial and METC Needs

Publications and Presentations. Eight quarterly progress reports were prepared during the course of this study in addition to the three volume final report. Also, ten theses or dissertations have been prepared or were in the process of being prepared at the time this final report was written. Eight papers were published in technical journals based on this work while other papers based on the work of Sowa (1987), Nichols (1987), Cope (1987), Smith (1987), Baxter (1987), Christensen (1987), and Rasband (1987) were in preparation for journal publication. Six technical presentations were made to report results from this gasification study.

Detailed Data Book. A Data Book (Smoot and Christensen, 1985) was prepared for the U.S. Department of Energy under Contract No. DE-AC21-81MC16518 to provide a convenient and reliable source of data for model evaluation. Errors were located, noted and subsequently corrected, and two new data cases were added to the Data Book. A revised edition of the Data Book is included as Volume 3 of this report.

Seven organizations have acquired PCGC-2 during the period of this contract, one has acquired 1-DICOG, and several others have inquired and are in the process of obtaining one or the other of the codes. The user's manual for PCGC-2 was revised, a new version of PCGC-2 was released for distribution, and plans were initiated for forming a user's group. A formal licensing agreement and policy for code distribution were also developed. The updated code, 87-PCGC-2, was placed at METC.

NOMENCLATURE

<u>Symbol</u>	<u>Definition</u>
A	Pre-exponential factor, area, constant
$AVE_{i,j}, AVW_{i,j}, AUP_{i,j}$	Coefficients of discretized axial velocity momentum equation at node i,j
$AVN_{i,j}, AVS_{i,j}, AVP_{i,j}$	Coefficients of discretized radial velocity momentum equation at node i,j
C	Coal (chemical symbol)
C_p, C_{NB}	Coefficients of discretized equation at node p
c	Coal (mass), heat capacity
E	Activation Energy
f	Fraction primary gas/total gas
g	Einstein function
I	Inertial under-relaxation factor
i	Element subscript
k	Reaction rate coefficient
n	Total number of increments
$P_{i,j}$	Pressure at node i,j
q	Heat transfer rate
R	Universal gas constant, Lagrangian auto-correlation function
r	Reaction rate
r	Under-relaxation factor
$r_{i,j}$	Radial distance for node i,j
S	Char (chemical symbol)
S_p	Source term of discretized equation at node p
T	Temperature
t	Time, characteristic time
u	Velocity
$u_{i,j}$	Axial velocity component at node i,j
V	Volatiles (chemical symbol)
v	Volatile (mass)
$v_{i,j}$	Radial velocity component at node i,j
w	Mass fraction
x,y,z	Coordinate directions
Y	Fractional volatile yield

<u>Symbol</u>	<u>Definition</u>
y	Mass fraction
z	Arbitrary argument
γ	Fraction window gas/total gas
Δ	Discrete difference
Δr	Radial width of p-cell i,j
Δx	Axial length of P-cell i,j
ϵ	Error term, eddy diffusivity
n	Fraction coal off gas/total gas
θ	Blowing factor
μ	Element atomic weight
ρ	Correlation coefficient
σ	Variance
τ	Time
ϕ_p^i	Variable ϕ at node p at iteration i
Σ	Summation
—	Mean property
a	Mass atomic weight

Subscripts

1,2	Reaction path 1 or 2, fractions 1,2
a	Ash
g	Gas
i	Element, data point i
P	Particle, constant pressure
ra	Radiation
rx	Reaction
T	Temperature
v	Volatiles, constant volume

Superscripts

n	Total number of
p	Primary input feed stream
s	Secondary input feed stream
t	Turbulent

Superscripts

w	Window purge input feed stream
l	Local property in flame
'	Arbitrary, fluctuating component
^	Predicted

I. INTRODUCTION AND SCOPE

Background

The large energy requirements of our country, the necessity of importing a significant fraction of our petroleum fuels, and the political and economic uncertainties caused by these imports require that the U.S. continue to develop alternate energy sources. Synthetic fuels derived from coal presents one of the most viable options for reducing our country's dependence on foreign oil and for supplying future energy needs. Gasification is a particularly attractive energy alternative because a single process can lead to electrical power, synthetic gas, or liquid fuels. The immediate application of gasification seems best for combined cycle power generation, as evidenced by EPRI, TEXACO, and Southern California Edison commitments to the Cool Water Project (e.g. Clark and Shorter, 1986) and the DOW (e.g. Fisackerly and Sundstrom, 1986) and SHELL (e.g. Perry and Nager, 1986) gasification process developments. Combined cycle entrained gasification shows promise of electric power production at costs competitive with conventional methods and with significantly lower pollutant emissions. Further, smaller units show promise of coming on-line quickly without large working capital expense. Even with this interest in entrained gasification technology, basic information on process variables and mechanisms, and on process modeling and control is very limited. Consequently, research on advanced coal technologies such as entrained coal gasification is a vital element in the development of this energy alternative.

Work has been conducted at this laboratory towards understanding the effects of mixing and reaction in an entrained gasifier (Smoot and Hanks, 1977; Smoot, et al., 1980; Hedman, et al., 1981; 1984; 1985; Skinner, et al., 1980; Price, et al., 1983; Lewis, et al., 1982; Highsmith, et al., 1985; Anderson, 1983; Soelberg, et al., 1985; Glassett, 1984; Nichols, 1985; Brown, et al., 1985). This study (fifth phase) was started in March of 1985. In four earlier phases of the program (ERDA Contract No. E(49-19)-1767, DOE Contract No. EF-77-S-01-2666, DOE Contract No. DE-AC21-80MC14380, and DOE Contract No. DE-AC21-81MC16518) the laboratory-scale entrained-coal gasifier was designed, constructed, and used to make coal gasification measurements at atmospheric pressure with four coal types, and at elevated pressure with a Utah bituminous coal (Smoot and Hanks, 1977; Smoot, et al., 1980; Hedman, et al., 1981; 1984; 1985). Gasifier tests to determine optimum operating conditions and to obtain detailed maps of local gas and particle composition and mass flux data from inside the gasifier were completed. Variables investigated included steam/oxygen/coal ratios, coal particle size, gasifier injector configuration, preheat temperature, secondary/primary mass flow and velocity ratios, and the partitioning of the O_2 between primary and secondary jets. One-dimensional and two-dimensional entrained-coal gasifier computer models were also completed (Smoot and Hanks, 1977; Smoot, et al., 1980; Hedman, et al., 1981; 1984; 1985; Smoot and Hedman, 1978; Smoot, et al., 1979; Smoot, et al., 1981; Smoot, et al., 1983) which can be used to describe the operation of entrained-coal reactors. The two-dimensional model, which is referred to as PCGC-2, is a generalized, axisymmetric code for turbulent, reacting pulverized-coal systems which includes a description of the turbulent fluid motion. Further, cold-flow jet mixing experiments were completed to provide fluid property measurements to support model development and validation. The results have

been applied to industrial needs through publication of reports and publications and through presentation of several technical seminars.

Project Objectives and Scope

The general purpose of this research program was to develop a basic understanding of the physical and chemical processes in entrained coal gasification and to use the results to further develop a gasification computer model. The first of three specific tasks was to make gasifier measurements, which included the collection and analysis of in-situ gasifier data at elevated pressure with three additional coal types, the design, construction, and testing of new coal/oxygen/steam injectors, the collection of supporting data from cold-flow studies, and the investigation of the feasibility of using laser-based diagnostic instruments to make measurements in coal flames. The second task was to refine the two-dimensional gasifier model, which includes the use of new coal devolatilization and char oxidation data in predictions, the development of improved numerical methods, an improved treatment of particle dispersion effects, and validation of the model through comparison of predictions with experimental results. The third task was to transfer technical advances to industry and to METC through technical seminars, production of a detailed data book, and code placement. Thus, the three tasks identified and incorporated into the project study were: Task 1 - Entrained Coal Gasification Measurements; Task 2 - Gasification Modeling; and Task 3 - Application to Industrial and METC Needs. Task statements follow for each.

Task 1 - Entrained Coal Gasification Measurements

Entrained coal gasification experiments were to be carried out: 1) to make parametric variation tests and mapping tests with Wyoming subbituminous, North Dakota lignite, and Illinois No. 6 bituminous coals at elevated pressure; 2) to investigate the effect of injector design on reactor performance; 3) to improve the understanding of gas fluid mechanics in the gasifier through a series of cold-flow measurements; and 4) to investigate the application of advanced laser diagnostics in the laboratory gasifier. The four subtasks that address each of these areas are discussed below.

Subtask 1.1 - Elevated Pressure Testing with Additional Coal Types. Parametric variation tests and mapping tests with the Utah bituminous coal at elevated pressure had been completed during an earlier study (Hedman, et al., 1985). However, the effect of coal rank (type) had not been investigated at elevated pressure. Under this subtask, elevated pressure tests with Wyoming subbituminous coal, North Dakota lignite, and Illinois bituminous coal were to be conducted. These tests were to include parametric variation tests (with the sample probes near the reactor exit) where the effects of operating variables (O_2 /coal, steam/coal, coal type, operating pressure, and coal feed rate) were to be determined on coal (carbon) conversion, heat loss, cold gas efficiency, and species concentration measurements, including sulfur and nitrogen pollutants. Mapping tests were also to be completed with each coal type at a single set of operating conditions (coal feed rate, O_2 /coal ratio and steam/coal ratio) at two different elevated pressure levels for two of the coal types, and at a single elevated pressure but at two different sets of operating conditions for the third coal type. Where possible, predictions were to be made with the PCGC-2 code for comparison to the experimental results.

Subtask 1.2 - Coal/Oxygen/Steam Injector Characterization Tests. The design of the coal/oxygen/steam injector is one of the critical aspects of the successful design of an entrained-flow coal gasifier. In this part of the program, the effects of various different injector configurations on gasifier performance were to be investigated. Designs that were to be considered included injectors that produced both premixed and diffusion flames. The PCGC-2 code was to be used in the design of the injectors that were to be tested. The study required that parametric variation tests be performed on three different injector designs. The parametric variation tests were to include measurements at the reactor exit to determine coal burnout and species concentrations at various operating conditions. A single reactor map (local measurements at various radial and axial locations) was also to be obtained for each injector at a single elevated reactor pressure. Operating conditions (O_2 /coal, steam/coal ratios, and coal feed rates) were to be selected to determine the most information about the injector performance. From this study, a data base was to be obtained for injector design that would provide for code evaluation for very different injector designs.

Subtask 1.3 - Cold-Flow Jet Mixing Tests. A laser Doppler velocimeter (LDV) was to be used to obtain local mean axial and tangential and rms axial and tangential velocity data in a cold-flow facility that was to be operated at conditions that simulated the flows in the entrained flow gasifier. The LDV system was to be used to examine the effect of different levels of swirl in the jet mixing duct on mixing rates and flow patterns. These data were to be obtained to better understand the usefulness of various swirl parameters in characterizing swirling flow. The LDV system was also to be used to characterize the inlet velocity profiles, and to check for flow symmetry across the entire inlet. Mean and fluctuating velocities, turbulence intensities, swirl decay, and other parameters were also to be measured. The results were to provide additional data needed as input into the gasification code, and also provide data needed for code evaluation. Near the conclusion of the test program, the LDV system was to be modified to incorporate a second channel with different frequency and color of light. The use of the second laser channel at a different light frequency allows simultaneous measurement of a second gas velocity component that is orthogonal to the initial velocity component.

Subtask 1.4 - Advanced Diagnostic Instruments. There have been some major advances in advanced, laser-based diagnostic instruments in recent years that permit local velocity, temperature, and species concentrations to be measured without the disturbing influence of a mechanical probe. A minor task was included in this project to investigate the feasibility of incorporating some of these advanced diagnostic instruments into the coal gasifier. This task was expanded part way into the program to support the development and fabrication of a coherent anti-Stokes Raman spectrometer (CARS) instrument that would have the capability of making temperature and species concentration diagnostic measurements in a coal reactor. A separate DOE instrumentation grant (Grant No. DE-FG05-84ER75153) had been received by the laboratory to fund the development of such an instrument.

Task 2 - Gasification Modeling

The major thrust of this task was to further refine and improve the pulverized coal combustion and entrained coal gasification computer code

(PCGC-2), and use the code to describe the gasification process. Three subtasks were identified which are summarized in the following paragraphs.

Subtask 2.1 - Physical Submodel Improvement. The physical submodels in the PCGC-2 code (particle dispersion, coal devolatilization, and char oxidation) represent areas of code development where considerable improvement was sought. The particle dispersion submodel in the two-dimensional gasification code was to be reviewed, compared with other models reported in the literature, and modified to provide the best prediction of particle dispersion possible. This submodel has been one of the most restrictive components in the code. The modified submodel was to be evaluated by comparison with available nonreacting particle dispersion data, and further modifications were to be made based on the results of the evaluation. New coal devolatilization and char oxidation rate data from several different coals were to be used to perform gasification predictions. Rate measurements from different laboratories were to be compared and used in the gasification predictions.

Subtask 2.2 - Numerical Solution Efficiency. The two-dimensional gasification model was to be modified to decrease computational time requirements and numerical instability problems (oscillations in the predicted results from iteration to iteration). An adaptive grid routine was to be incorporated in the PCGC-2 code to optimize the grid locations. This was expected to speed convergence by reducing numerical instability as well as by increasing grid spacing in aft reactor regions. The two-dimensional code was to be examined and modified where possible to improve efficiency, readability, and transportability.

Subtask 2.3 - Model Evaluation. The two-dimensional code was to be evaluated by extensive comparison with experimental measurements of species concentration, temperature, and char burnout measurements from high-pressure gasifier tests of Task 1. Comparisons between predictions and experimental data were also to be made for results from injector/burner studies. At least one prediction was to be made for each experimental map obtained under Subtasks 1.1 and 1.2. Minor improvements were to be considered, where possible, to improve agreement. Parameter predictions of key model parameters were to be performed, although a complete sensitivity analysis was not to be performed due to computer limitations and code complexity. Where possible, parametric tests of input parameters (i.e., flow rates, coal types, etc.) were to be compared both qualitatively and quantitatively with corresponding experimental data.

Task 3 - Application to Industrial and METC Needs

The results of this study were to be communicated to METC and potential industrial users. Possible industrial applications were to be identified, and assistance was to be given in evaluation and implementation of the potential applications. Additional data were to be added to the Data Book, and the latest version of the code was to be placed at METC.

Subtask 3.1 - Technical Seminars. Detailed technical seminars which document the results of this study were to be presented at METC, at the annual contractor's meeting, and at selected technical conferences as required. Members of the BYU Industrial Panel were to meet once during the contract for an extensive review and evaluation of the program and results.

Subtask 3.2 - Detailed Data Book. The detailed data book prepared in the previous study (Smoot and Christensen, 1985) was to be revised as additional data sets were completed, and as additional data sets were found in the literature. This data book provides a summarized source of experimental data for rigorous evaluation of entrained coal gasification codes and is available for use by METC and industry. A revised version was to be submitted with the final report.

Subtask 3.3 - Code Placement. The latest version of the two-dimensional code (PCGC-2) was to be placed at METC. FORTRAN listings, users manuals, and example cases were to be supplied. On-site assistance at METC was to be provided in order to make the code functional and train the engineers in its use. The functional code was also to be placed for distribution with the National Energy Software Center (NESC).

II. TASK 1: ENTRAINED COAL GASIFICATION MEASUREMENTS

Introduction

Background

Entrained coal gasification is a relatively new technology when compared to the earlier fixed bed techniques. Entrained gasification is attractive because it has the potential of higher reactor throughput, and consequently lower cost, and it can use caking or agglomerating coals without plugging the reactor. An extensive survey of the early development of entrained coal gasifiers has been completed by Bissett (1978). While commercial entrained gasifiers exist, the basic principles of entrainment and reaction are not fully understood. Researchers at this laboratory have been investigating the physical and chemical mechanisms involved in entrained coal gasification. In previous gasification studies at the BYU Combustion Laboratory, the entrained flow gasifier was designed and constructed (Smoot and Hanks, 1977). Gasification tests at atmospheric pressure have been performed with four different coal types, and elevated pressure tests were performed with the Utah bituminous coal. Gas and particle samples were extracted from the gasifier and analyzed to determine the extent of gas mixing, particle dispersion and reaction, and the concentration of gaseous reaction products throughout the reactor (Smoot, et al., 1980; Hedman, et al., 1981; 1984; 1985).

Objectives

The general objectives of this study task were to: 1) make additional gasifier measurements at elevated pressure with three additional coal types, which includes the collection and analysis of in-situ gasifier data, 2) the design, construction, and testing of new coal/oxygen/steam injectors, which also includes the collection and analysis of in-situ gasifier data, 3) the collection of supporting data from cold-flow studies, and 4) the investigation of laser-based advanced diagnostic techniques that would be suitable for use in making in-situ measurements of temperature, and species concentration measurements in an entrained coal gasifier. The collection of test data could be used to evaluate computer codes. Specific details on the subtasks to be performed in Task 1 were summarized in Section I of this report.

Approach

Gasification Subtasks 1.1 and 1.2 used the existing entrained flow gasifier, which was designed, constructed, and operated during previous phases of the gasification program at BYU (Smoot and Hanks, 1977; Smoot, et al., 1980; Hedman, et al., 1981; 1984; 1985). However, it was necessary during this study to relocate the gasifier to the Combustion and Reactions Laboratory Building that was remodeled by Brigham Young University to specifically house the Combustion Laboratory reaction facilities. This relocation was not a specific part of this study, but it had a great impact on the study. While the facility was being relocated, considerable modification and improvement in the operation and control of the reactor was implemented. The modifications to the facility are discussed in a following section of this report.

The basic experimental approach used in the reactive tests was to obtain a particle-gas sample from inside the reactor using specially designed water-quenched sample probes. Particulate materials in the sample were separated and analyzed to determine the rate of particle mixing and reaction and also to determine the ash, volatile matter, and sulfur and nitrogen content. Reacting gas samples were analyzed to determine the concentration of such quantities as CH_4 , CO , CO_2 , and H_2 . This information provided direct measurement of the extent of coal gasification, and the extent of sulfur and nitrogen pollutant formation. Detailed information on local chemical composition also served to provide a data base for direct model comparison.

A modified laser system was used to obtain specific data on mean axial and tangential and rms axial and tangential velocities in a cold-flow facility that was operated at conditions that simulated the flows in the entrained flow gasifier. The results obtained provided additional data needed as input into the gasification code, and also provided data needed for code evaluation.

There have been some major advances in laser-based diagnostic instruments in recent years which allow local velocity, temperature and species concentration measurements to be made without the disturbing influence of a mechanical probe. A minor task was included in this project to investigate the feasibility of incorporating some of these instruments into the coal gasifier. This task was expanded part way into the program to support the development and fabrication of a coherent anti-Stokes Raman spectrometer (CARS) instrument that would have the capability of making temperature and species concentration diagnostic measurements in a coal reactor. A separate DOE instrumentation grant (Grant No. DE-FG05-84ER75153) had been received by the laboratory to fund the development of such an instrument.

Test Facility and Sample System

Entrained Coal Gasifier

The design and fabrication of the entrained coal gasifier has been described in detail elsewhere (Skinner, et al., 1980; Anderson, 1983, Sowa, 1987). A schematic of the gasifier is shown in Figure 1. The gasifier was designed to study entrained flow coal gasification processes up to 1800 kPa (250 psig). The reactor length and internal reactor volume were the same in this study as reported in the previous study (Hedman, et al., 1985). Argon gas was used to blanket the coal feeder, as a primary stream entrainment medium, and as a gas tracer. Helium gas was also available as a gas tracer in the secondary stream.

The facility was constructed with the capability of distributing or partitioning oxygen in any proportions between the primary and secondary streams. The oxygen was supplied from a bank of twelve, high-pressure, 6.2 cu.m gas cylinders (purity=99.6%). The primary oxygen stream was mixed with the argon coal mixture 13 inches above the reaction chamber entry point. Although primary oxygen preheat was available, it was not used. The secondary oxygen stream was mixed with steam in an electric heater 8 m from the reaction chamber. The secondary gas temperature was 300 K when steam was not used, and 454 K when steam was used. The later temperature represents the steam saturation temperature.

Figure 1. Schematic drawing of the BYU entrained flow laboratory-scale coal gasifier.

The reactor consisted of six, 30.5 cm sections and one 15.2 cm section, each with a 20 cm inside diameter. Each section was lined with 5 cm of refractory liner. The refractory liner was changed twice during the contract period, as problems with meltdown and slag attack were encountered. Sections were fabricated with observation ports to aid in observing flame ignition and reactor operation as well as to provide a mount for the traversing sampling probe. The observation ports were purged using either N₂, Ar or He gas. The reactor wall temperatures were monitored using K-type thermocouples (chromel/alumel) which were placed in the reactor wall at two different depths from the inside wall surface, 0.32 cm and 1.27 cm. A K-type thermocouple was also placed in the reactor exhaust to monitor exhaust gas temperatures. No attempt was made to shield or protect this thermocouple from radiation or deposit buildup or to correct the gas temperature.

The oxygen, argon and window port purge gas flowrates were all measured with choke flow nozzles. The steam flow rate was monitored using a Ramapo target meter.

Facility Modifications

As part of the relocation of the gasifier to the new laboratory building, several design modifications were undertaken. Ten major facility subsystems were modified during installation of the facility. The purposes of the modifications were to: 1) increase safety, 2) increase maximum operating capacity of the facility for greater operational flexibility, 3) improve accuracy of feedstream measurements, 4) improve pressurization control, 5) decrease complexity, and 6) increase process efficiency. A more detailed review of the facility modifications is contained in the dissertations of Sowa (1987) and Nichols (1987) and the thesis of Cope (1987).

Exhaust System. The exhaust system of the gasifier was completely redesigned to take advantage of the increased space in the Combustion and Reactions Laboratory Building, and improve the pressure control system. The method of pressure control was changed from a bladder valve on the exhaust gas line and a cyclic water dump to the sewer on the scrubber to throttle control valves on both the exhaust gas line and the sewer connection. The packed column scrubber was changed to a wet venturi scrubber-cyclone disengager to separate the water and particulate from the exhaust gas. A National Airoil gas flare was added to completely oxidize all of the gasification products before being discharged to the atmosphere. This change greatly simplified the exhaust system and the requirements for maintenance. A target meter was purchased to replace the turbine meter, however, manufacturing and delivery time precluded the use of the target meter in the current study.

Coal Feed System. The coal feed system was modified to increase the maximum coal feed rate from 35 kg/hr to 100 kg/hr, and to improve the accuracy and control of the coal feed rate. This change involved modifications of auger gearing and the suspension of the feeder vessel from a balance beam (Nichols, 1987). A schematic of the coal feed system is shown in Figure 2.

Numerous additional modifications were made to the coal feeder vessel to improve its operation and its maintainability. These modifications included: 1) replumbing the argon blanket and argon pickoff points to assure more uniform partitioning of the argon; 2) replumbing the feeder purge line,

Figure 2. Schematic of the coal feeder/balance beam assembly.

3) installation of a filter at the purge port to prevent the dumping of coal during purging operations; 4) replumbing the feeder fluff and quick pressurization ports to improve the control of feeder vessel pressurization; 5) remanufacture the coal stirrer from hardened steel; 6) installation of grease ports to the stirrer shaft; 7) remanufacture of the coal intramitter shaft to improve maintainability.

Quench Water Supply System. In order to quench the increased volume of exhaust gas due to increased coal feed rates, a 76 μ m (20 gpm) diaphragm pump was purchased to replace the 23 μ m (6 gpm) piston pump that was used during the previous BYU studies. During all gasifier firings that involved pressures above 2 atm, the water pumps were necessary to boost the needed quench water pressure above the water supply pressure. The 23 μ m (6 gpm) piston pump was installed on the deionized water supply line. Deionized water was used in the water-quenched sample probes. The use of deionized water for char-gas sampling in the reaction chamber was not employed during previous BYU studies at pressures above 2 atm.

Oxygen, Argon, Nitrogen and Helium Supply Systems. All reactor facilities that are housed in the Combustion and Reactions Laboratory Building were tied into a common gas supply system. This change simplified the gas supply systems without sacrificing accurate accounting of gas usage among the different experiments. A gas cylinder storage room was constructed in the laboratory building to increase cylinder storage capacity, and to improve safety and organization.

Steam Supply System. Only the method of measuring the steam flow rate was modified on the steam supply system. The previously used straight-edged orifice and d-p cell were replaced with a Ramapo Target Meter that was manufactured for steam service. The target meter greatly enhanced the overall accuracy of the measurement of steam feed rates. The Foxboro electronic d-p cell that was previously used to measure steam feed rates was moved to the exhaust gas system to measure water levels in the water-solid collection tank below the cyclone disengager.

Feedback Control Systems. During previous studies, feedback control was used on the oxygen, preheat air and steam supply lines. The feedback control was removed from the all these lines and replaced with open loop control. This change was made to decrease the complexity of the feedback loops and to remove the oscillatory response of the feedback controllers that could not be tuned out of the controllers while still maintaining the wide range of gas flow rates needed during each firing.

Sample Probe and Collection System. The previous gasification study used two different sample trains depending on whether the samples were to be taken at atmospheric or elevated pressures. The sample train was simplified so that all test conditions could be handled with one sample system. In-situ gasification samples were collected with a water-quenched probe similar to the probes used by Thurgood (1979) and Skinner (1980). The probe, as shown in Figure 3, was constructed of stainless steel. The thickness of the outer wall of the probe was increased over previous probe designs. This resulted in greater strength and longer lasting probes. Sample flow was achieved by maintaining a small pressure differential (1-2 psi) between the gasifier and the inner tube of the probe.

Figure 3. Schematic of traversing probe for gasifier.

The sample probe was mounted on a remote control traversing mechanism (Anderson, 1983). This traverser could be attached at any one of the several ports, each port being at a different axial location. The traverser allowed the probe to be moved radially between the reactor centerline and the reactor wall.

The water-quenched sample was withdrawn from the reactor with the probe to a separation system, as shown in Figure 4. This system was designed and built like earlier systems (Highsmith, 1982). The components were located on the control panel, outside of the gasification test bay. All components were of stainless steel to minimize the potential for the sample to change chemically. The sample first entered a vessel (disengager) where the gas phase was separated from the condensed phase (liquid and char). The gas from this first disengager passed through a cooling coil immersed in a water-ice bath, and any further condensate separated by a second disengager. The gas phase was filtered (2 μm filter), after which it was available for: 1) on-line NO_x , CO and CO_2 analyses, and 2) collection in a sample bag for subsequent chromatographic analyses.

The condensed phase was collected in a sample jar and was filtered later to separate the char from the liquid. The char was then dried in an oven at 105°C for 1.5 hours. In this manner, each in-situ gasifier sample was separated into three phases (gas, liquid, solid) for subsequent elemental and species analyses.

Preheat System. Several components of the ignition and preheat system were modified to provide consistent ignition and safety. A choke flow nozzle was added to the natural gas supply line to measure natural gas feed rates. A rotameter was added to the hydrogen line to the spark ignitor to measure H_2 feed rates. A RIX Model HG-3, "Hom-Gas" encapsulated natural gas compressor was used to fill 4 gas cylinders with 32.4 cu. m of natural gas at 2200 psig before every firing. This modification allowed the coal flame to be stabilized at elevated pressure with pressurized natural gas. The natural gas line was rerouted to enter the reaction chamber through the primary stream. Previously the natural gas was introduced through the H_2 -air ignitor entry port. Figure 5 shows the previous methods of introducing natural gas and air to the combustion chamber as well as the method used during this study. In both studies, the preheat combustion air or oxygen was introduced through the secondary stream of the injector. The rerouting of the natural gas stream allowed for much simpler ignition than the previous arrangement.

Refractory. A desire to reduce the overall facility heat loss, and to reduce refractory erosion necessitated modification of the refractory lining previously used. Several different combinations of commercial refractories were tried without success. Eventually, Jade Pak-88-P-Plus, a chromium containing refractory with high service temperature was installed in the reactor.

This new refractory lessened the slag attack in the highly reducing gasification environment. This refractory also had a higher thermal conductivity (compared to previous combinations that were tried) which protected it from wall paper temperatures greater than the maximum service rating. An insulating ceramic paper, 0.32 cm thick was installed between the ceramic liner and the reactor shell to lower the overall wall thermal

Figure 4. Gasifier sample collection system.

Figure 5. Schematic diagram highlighting feedstream modifications for ignition and preheating the gasifier.

conductivity, and lessen the heat loss. The ceramic paper was a Fiberfrax product from Carborundum. This combination of refractory and ceramic paper lasted throughout the remainder of the experimental work. The average wall temperatures were comparable to the wall temperatures of previous studies; however, the erosive wear of the refractory appeared to be much less than previously experienced.

Injector. The primary tube assembly was redesigned to increase safety by reducing the threat of flashback, and to increase flexibility when changing from one injector type to another.

Facility Limitations

Throughout the course of the experimental work, several additional facility limitations were discovered. Most of these limitations can be modified in future studies. The limitations are summarized in Table 1.

TABLE 1
FACILITY LIMITATIONS FROM EXPERIENCES DURING THE
EXECUTION OF THE CONTRACT WORK

<u>Limitation</u>	<u>Constraint</u>
Maximum coal feed rate at atmospheric pressure: 50 kg/hr	Capacity of sewer control valve
Maximum coal feed rate at elevated pressure: 120 kg/hr	Size of coal feed auger
Maximum coal feed rate for 1 hour operation: 70 kg/hr	Size of coal feed hopper and oxygen manifold capacity
Maximum coal feed rate for *Wyoming coal at elevated pressure: 50 kg/hr	Above 50 kg/hr, the heat release is too great for the refractory
Maximum operating pressure for operation with a premixed Utah bituminous coal flame: 5 atm	Above 5 atm pressure the flame was too close to the injector causing injector meltback
Maximum operating pressure for operation with a Utah bituminous coal diffusion flame: 6 atm	Product volumetric flowrate too small for safe throttling
Maximum operating pressure: 17 atm for O ₂ /coal ratios between 0.7 and 1.0.	Reactor vessel pressure rating

Test and Analysis Procedures

The procedures used to operate the gasifier at atmospheric pressure have been detailed by Skinner (1980), Highsmith (1982), and Soelberg (1983), Brown (1985) and at elevated pressure by Anderson (1983). Similarly, analysis procedures have been discussed in detail by Price (1980), Burkinshaw (1981), Highsmith (1982) and Nichols (1985). Some modifications in these analysis and operating procedures were implemented in this study. A brief summary of these testing procedures is contained in Appendix D. Additional procedural details can be found in Sowa (1987) and Nichols (1987).

Subtask 1.1 - Elevated Pressure Testing with Additional Coal Types

Coal Selection and Properties

Previous tests conducted in this laboratory by Brown (1985) and Azuhata et al. (1986a and 1986b), supported by DOE Contract No. DE-C21-81MC16518, investigated the effects of coal type on entrained-coal gasification at atmospheric pressure. The coals selected for Brown's study included North Dakota lignite (ND), Wyoming subbituminous coal (WYO), and Illinois No. 6 bituminous coal (ILL). Azuhata's tests used Utah high volatile bituminous coal (UT). Quantities of North Dakota lignite, and Illinois No. 6 bituminous coal remaining from Brown's tests were adequate for use in this study. Approximately 1.75 tons of Wyoming subbituminous coal were obtained from the Black Thunder Mine in Wright, Wyoming to be used in conjunction with these two coals. Samples of all three coals were sent to Commercial Testing and Engineering Company in Denver Colorado for analysis. The results of these analyses are presented in Table 2.

All coal samples used in this study were ground to about 50 μm in BYU's MikroPul #1 HS bench-scale pulverizer. Though the resulting mass mean diameter of the Illinois bituminous coal was about 5 μm lower than those of the Wyoming subbituminous and North Dakota lignite, as shown in Figure 6, the effort to obtain near equal size distributions and mass mean diameters was otherwise successful.

Test Program

A series of parametric variation tests, and spatially resolved mapping tests were conducted to determine the effects of coal rank on entrained-coal gasification performance at elevated pressures. The parametric variation tests were to evaluate the effects of operating variables in gasification performance. The mapping tests were to collect data from within the reactor to provide local data for model comparison. Both of these test series were conducted with a premixed flame (coal and oxygen injected through the primary feed line) exclusively.

For the parametric variation tests, the sample probe was positioned on the centerline at the gasifier exit. Tests were then conducted for each of the three coals at each of two different levels of coal feed rate, O_2 /coal ratio, steam/coals ratio, and operating pressure. An objective of the parametric variation study was to explore a range of these variables on carbon conversion and product species composition. Desired operating levels were

TABLE 2

PROXIMATE AND ELEMENTAL ANALYSES OF THE NORTH DAKOTA LIGNITE,
WYOMING SUBBITUMINOUS AND ILLINOIS BITUMINOUS TEST COALS

<u>Coal Type</u>		<u>Proximate Analysis (wt. %)</u>		<u>Ultimate Analysis (wt. %)</u>		
		<u>As Received</u>	<u>Dry Basis</u>		<u>As Received</u>	<u>Dry Basis</u>
North Dakota Lignite	Moisture	34.4	--	Moisture	34.4	--
	Ash	6.5	9.9	Carbon	41.0	62.5
	Volatiles	29.6	45.2	Hydrogen	2.7	4.1
	Fixed Carbon	29.5	44.9	Nitrogen	0.5	0.8
				Chlorine	0.1	0.1
	Higher Heating Values (Btu/lb)	6685	10192	Sulfur	0.7	1.1
				Ash	6.5	9.9
			Oxygen	14.1	21.5	
Wyoming Subbituminous	Moisture	24.8	--	Moisture	24.8	--
	Ash	6.0	7.9	Carbon	51.8	68.8
	Volatiles	33.8	44.9	Hydrogen	3.7	4.9
	Fixed Carbon	35.5	47.2	Nitrogen	0.6	0.8
				Chlorine	0.0	0.1
	Higher Heating Values (Btu/lb)	8990	11948	Sulfur	0.3	0.3
				Ash	6.0	7.9
			Oxygen	13.0	17.2	
Illinois Bituminous	Moisture	10.9	--	Moisture	10.9	--
	Ash	11.3	12.6	Carbon	58.6	65.8
	Volatiles	35.0	39.3	Hydrogen	4.2	4.7
	Fixed Carbon	42.9	48.1	Nitrogen	1.1	1.2
				Chlorine	0.0	0.1
	Higher Heating Value (Btu/lb)	10497	11780	Sulfur	3.6	4.0
				Ash	11.3	12.6
			Oxygen	10.3	11.6

Figure 6. Measured particle size distributions.

coal feed rates of 25 and 75 kg/hr, O_2 /coal ratios of 0.85 and 1.0, steam/coal ratios of 0.0 and 0.3, and operating pressures of 5.5 and 10 atm. Subsequent tests conducted with the Wyoming coal however, indicated that these operating levels were impractical because of limitations of the gasification system (see Table 1). The capacity of the coal feeder was inadequate for maintaining a coal feed rate of 75 kg/hr throughout the duration of a run. A coal feed rate of 25 kg/hr was too low to prevent a flashback at an operating pressure of 10 atmospheres, and thus was raised to 33 kg/hr. The thermal capacity of the gasifier ceramic dictated that a coal feed rate of 50 kg/hr and an O_2 /coal ratio of 0.85 be considered as maximum values. A value of 0.70 was set for the lower O_2 /coal ratio. It was decided to consider the moisture entering the gasifier to be solely a property of coal rank, so the steam/coal ratio was fixed at 0.0 and eliminated as a variable. A summary of the test variable levels that were used for each of the three coals during these tests is shown in Table 3.

TABLE 3
DESIGN VALUES FOR PARAMETRIC
VARIATION TEST MATRIX

<u>Coal Feed Rate (kg/hr)</u>	<u>O_2/Coal Ratio (kg/kg)</u>	<u>Operating Pressure (atm)</u>	<u>Axial Position (cm)</u>	<u>Radial Position (cm)</u>
33	0.70	5.5	173	0
33	0.85	5.5	173	0
33	0.70	10.0	173	0
33	0.85	10.0	173	0
50	0.70	5.5	173	0
50	0.85	5.5	173	0
50	0.70	10.0	173	0
50	0.85	10.0	173	0

The spacially-resolved mapping tests were conducted by operating the gasifier at each of two sets of constant operating conditions. Before each test, the sample probe was located at a fixed axial position inside the gasifier. During a test, the probe was traversed radially to various sample positions between the gasifier centerline and wall. Only centerline (0 cm radial position) samples were taken at the 173 cm axial position, because previous elevated pressure tests conducted by Azhuta (1986b) showed no significant variation with radial position at this axial position. The operating conditions, and sample probe positions used during this test series are listed below in Table 4.

TABLE 4

DESIGN TEST CONDITIONS FOR SPACIALLY
RESOLVED MAPPING TEST MATRIX

Coal Type	Coal Feed Rate (kg/hr)	O ₂ /Coal Ratio (kg/kg)	Operating Pressure (atm)	Axial Positions (cm)	Radial Positions (cm)
ND	33	0.85	5.5	22, 52, 83, 173	0, 2, 4, 6, 8
ND	33	0.85	10.0	22, 52, 83, 173	0, 2, 4, 6, 8
WYO	33	0.85	5.5	22, 52, 83, 173	0, 2, 4, 6, 8
WYO	33	0.85	10.0	22, 52, 83, 173	0, 2, 4, 6, 8
ILL	33	0.85	5.5	22, 52, 83, 173	0, 2, 4, 6, 8
ILL	50	0.85	5.5	22, 52, 83, 173	0, 2, 4, 6, 8

Parametric Variation Test Results

The results of the parametric variation tests for each of the three coals are summarized in Appendix A. The safe operating limits of coal feed rate and O₂/coal ratio were determined while using the Wyoming subbituminous coal. For this reason, coal feed rates of 63, 85, and 111 kg/hr, and O₂/coal ratios ranging from 0.56 to 1.27 were obtained with the Wyoming coal. The results of the 85 and 111 kg/hr tests are reported in Appendix A., but will not be included in the following analysis because of their limited nature and great differences from the remainder of the parametric variation tests. The test values of coal feed rate and O₂/coal ratio reported in Appendix A differ from those shown in Table 3, because of difficulties in reaching and maintaining the desired coal feed rate.

Data Accuracy. The accuracy of the data obtained for Subtask 1.1 is summarized below in Table 5. Further detail on the data accuracy is given in the discussion of Subtask 1.2.

Carbon Conversion. Exit plane carbon conversion values as a function of O₂/coal ratio, have been fit by a least squares line for each of the three coals in Figures 7(a), 8(a) and 9(a). These figures show that carbon conversion increases with increasing O₂/coal ratio for all three coals. The levels of carbon conversion obtained at a coal feed rate of approximately 33 kg/hr and an operating pressure near 10 atm are at or near the maximum conversions obtained for each of the coals. This is to be expected, since this set of operating conditions produces the lowest injection velocity and the highest residence time in the gasifier. At these same conditions however, the change in carbon conversion with increasing O₂/coal ratio is only slightly positive or even negative. This is attributed to the fact that these conditions of minimum coal feed and maximum operating pressure approach an unstable region of gasifier operation. The existence of this unstable mode of operation is supported not only by the observed inconsistencies between these data and those obtained at other operating conditions, but also by the primary feed tube flashbacks experienced at these conditions during this and the

TABLE 5
ACCURACY OF MEASURED AND CALCULATED VALUES

<u>Measurement</u>	<u>Standard Deviation %</u>	<u>Measurement</u>	<u>Standard Deviation %</u>
<u>Solids:</u>		<u>Major Gas Species:</u>	
C	0.72	H ₂	0.75
H	0.17	Ar	0.15
N	0.19	O ₂	0.06
S	0.05	CO ₂	0.59
Ash	0.30	N ₂	0.94
O	1.00	CH ₄	0.04
Moisture	0.50	CO	0.88
<u>Calculated Value</u>		<u>Standard Deviation %</u>	
Exhaust water mole fraction		4.42	
Coal carbon conversion		1.75	
Coal hydrogen conversion		1.22	
Total coal conversion		1.60	
Cold gas efficiency		0.01	
Reactor heat loss		0.02

Figure 7. Effect of O_2 /coal ratio and operating pressure on carbon conversion, and cold gas efficiency with North Dakota lignite.

Figure 8. Effect of O_2 /coal ratio and operating pressure on carbon conversion and cold gas efficiency with Wyoming subbituminous coal.

Coal Feed Rate (kg/hr)	Operating Pressure (atmospheres)	
	5.3-6.4	9.6-10.1
30.7 - 31.7	◆	◇
40.1 - 41.3	▲	▴
50.6	■	

Figure 9. Effect of O₂ /coal ratio and operating pressure on carbon conversion and cold gas efficiency with Illinois bituminous coal.

Azuhata (Azuhata et al., 1986b) studies. These data inconsistencies are observed not only for carbon conversion, but for all other results that will be discussed. For this reason, the data obtained at an operating pressure of 10 atm and a coal feed rate of 33 kg/hr are reported in Appendix A, but are not shown on Figures 7-9, 11 and 12.

In general, the North Dakota lignite has the highest conversion, followed by the Wyoming and then the Illinois coals. Similar coal rank effects were observed by Brown (1985), and are attributed to the increase of inherent oxygen in the coal, and to the increase in char reactivity as rank decreases.

Previous studies conducted by Azuhata (Azuhata et. al., 1986b) found an increase in carbon conversion, with increased operating pressure, for a diffusion flame and an O_2 /coal ratio greater than 0.8. The same effect was not observed when using a premixed flame, possibly because of the limited nature of the Azuhata premixed flame data. While Azuhata was able to conduct tests with the diffusion flame at an operating pressure of 10 atm, problems with primary feed tube flashbacks prevented him from conducting premixed flame tests at pressures exceeding 5 atm. Premixed flame data were obtained in this study after reducing the inner diameter of the primary feed tube, thereby reducing the incidence of flashbacks. Figures 7(a), 8(a) and 9(a) show, for each of the three coals (while using a premixed flame), a general increase in carbon conversion as operating pressure increases. This effect can be attributed to the increase in residence time as operating pressure increases.

The effect of coal feed rate on carbon conversion is not readily apparent from these figures. The Wyoming data show a decrease in carbon conversion as the feed rate of coal is increased from ca 33 to ca 50 kg/hr, followed by an increase in conversion as the feed rate is increased to values greater than 50 kg/hr. The Illinois data show increased carbon conversion as the coal feed rate is increased from ca 33 to ca 50 kg/hr, while the North Dakota lignite data show both increased and decreased conversion with increased coal feed.

Heat Loss. The calculated fractional heat loss for each test is listed in Appendix A. The average fractional heat loss as a function of average coal feed rate is plotted for each coal in Figure 10.

This figure shows that fractional heat loss in the gasifier consistently decreased with increasing coal rank. This result is partially explained by the increase in heating value as rank increases. A decrease in heat loss is also shown for the lignite and subbituminous coal as both the coal feed rate and the operating pressure increase. Similar results were observed by Brown (1985), and were attributed to a nearly equal amount of lost heat, that represents a lower fraction of total available heat as the heat release rate increases with feed rate, and residence time. The limited data set for the bituminous coal also shows a decrease in heat loss with increasing coal feed rate, at 10 atm pressure. The 5.5 atm data show the opposite trend, increased heat loss with increased coal feed rate, for reasons not identified. No clear effect of O_2 /coal ratio on heat loss was identifiable. More discussion on heat loss is reported in Cope (1987) and Sowa (1987).

Cold Gas Efficiency. Cold gas efficiency (ratio of cold energy in product gas to input energy in coal) is shown as a function of O_2 /coal ratio, for the three coals, in Figures 7(b), 8(b), and 9(b). As coal rank increases,

Figure 10. Gasifier heat loss as a function of coal feed rate for three coals.

or as O_2 /coal ratio decreases, cold gas efficiency generally increases. Since cold gas efficiency is dependent on the heating value of the effluent gas, which in turn is strongly dependent on CO and H_2 levels, a positive correlation between coal rank and effluent concentrations of either or both CO and H_2 would be expected. This correlation will be discussed further in the section dealing with effluent species concentrations. The decreased cold gas efficiency as O_2 /coal ratio increases is due to the increased production of CO_2 , as more oxygen is available for reaction. The data obtained at a coal feed rate of ca. 33 kg/hr, and an operating pressure of 10 atm are not shown in these figures, for the reasons previously stated, but are listed in Appendix A. At these conditions, a less marked or even an opposite trend from the data collected at the other operating conditions was observed.

It was also observed that at a given O_2 /coal ratio, cold gas efficiency increases with increasing pressure, and generally increases with increasing coal feed rate. The increase in cold gas efficiency with increasing pressure, is related to the decrease in gasifier heat loss as operating pressure increases.

CO/ CO_2 Ratio. Figures 11(a,b, and c) show the exit CO/ CO_2 ratio as a function of O_2 /coal ratio for the lignite, subbituminous coal, and bituminous coal, respectively. The exit CO/ CO_2 ratio increases with decreasing O_2 /coal ratio, or with increasing coal rank. The coal properties listed in Table 2 show that the amount of oxygen inherent to the coal increases as coal rank decreases. These two results are therefore due to the same effect, an increase in CO_2 production as available total oxygen increases. This increase in CO_2 can occur partially at the expense of CO, decreasing the CO/ CO_2 ratio even more significantly. The results obtained for the low coal feed rate, high pressure case were again less pronounced or even opposite those observed for the other cases.

Within the design range of O_2 /coal ratio (0.70-0.85), CO/ CO_2 ratio increases with both increasing operating pressure and increasing coal feed rate. These effects could be related to decreased heat loss.

H_2 Concentration. Effluent mole % H_2 as a function of O_2 /coal ratio is shown for each of the three coals in Figure 12(a,b, and c). Effluent H_2 concentrations are seen to vary only slightly as a function of coal type. With all three coals, this concentration decreases as O_2 /coal ratio increases. Comparison of the effluent gas mole percentages of H_2 and H_2O show that H_2O concentrations tend to increase and H_2 concentrations decrease, as available O_2 increases. This indicates that the decrease of H_2 as O_2 /coal ratio increases is due to the oxidation of H_2 to water. The ca. 33 kg/hr coal feed rate data, at both levels of operating pressure, are consistent with these trends (see Appendix A). At a fixed O_2 /coal ratio, effluent H_2 concentration generally increases as both operating pressure and coal feed rate increase.

Mapping Tests with the North Dakota, Wyoming, and Illinois Coals

Sample Locations. In an effort to better understand the gasification process at high pressure, radial and axial profiles were obtained from inside the gasifier for the three coal types. A complete radial profile consists of samples taken at 0, 2, 4, 6, and 8 cm from the gasifier centerline. Complete

Coal Feed Rate (kg/hr)	Operating Pressure (atmospheres)	
	4.9-6.4	8.6-10.4
23.1 - 35.5	●	◆
38.6 - 43.5	▲	▴
46.7 - 53.0	■	□
64.8 - 67.2	▲	▴

Figure 11. Effect of O₂/coal ratio and operating pressure on CO₂ concentration with a) North Dakota lignite, b) Wyoming subbituminous coal, and c) Illinois bituminous coal.

Coal Feed Rate (kg/hr)	Operating Pressure (atmospheres)	
	4.9-6.4	8.6-10.4
23.1 - 35.5	●	◆
38.6 - 43.5	▲	▴
46.7 - 53.0	■	□
64.8 - 67.2	▲	▴

Figure 12. Effect of O_2 /coal ratio and operating pressure on H_2 concentration with a) North Dakota lignite, b) Wyoming subbituminous coal, and c) Illinois bituminous coal.

radial profiles were attempted at axial positions of 22, 52, and 83 cm from the gasifier inlet. The radial profile obtained at the 22 cm axial position lacks the centerline sample. This sample generally was unobtainable because the sample probe plugged in such close proximity to the gasifier inlet. Only centerline samples were taken at the gasifier exit (173 cm.). Test conditions for the profile tests were summarized in Table 4.

Test Results. The major gas species that were measured during the profile tests included Ar, CO, CO₂, H₂, CH₄, O₂, and N₂. Measured pollutant species were NO, HCN, NH₃, H₂S, COS, CS₂, and SO₂. The gas temperature at the gasifier exit was measured by means of a thermocouple. While these temperatures identify trends within the gasifier, their magnitudes are incorrect because no adjustments were made to account for the effects of char deposition, radiation, or conduction. An ash balance method was used to compute elemental conversion values, and mass balance closures (mass leaving the gasifier/mass entering the gasifier). Inconsistencies in the data obtained during several of the tests led to unrealistic results, possibly due to poor mass balance closure. Such results have been excluded from further analysis, and only those cases with a mass balance closure within the range of 0.85 to 1.15 are included in Appendix B and the following discussion.

Reactor maps of carbon conversion, CO concentration, CO₂ concentration, and H₂ concentration were constructed for each test series by double interpolation of the radial and axial profiles according to the method employed by Soelberg (1983) and Brown (1985). The design operating conditions for the maps are O₂/coal ratio of 0.85, steam/coal ratio of 0.0, operating pressures of 5.5 and 10 atmospheres, and a coal feed rate of 33 kg/hr (except for the series of 55 kg/hr tests with the Illinois No. 6 coal). Excluded from these maps are the inaccurate data points described earlier, as well as those points that were obtained at operating conditions greatly different from design conditions. Such exclusions impact chiefly on the elevated pressure tests with North Dakota lignite, because no suitable data points were obtained at the 52 cm axial position. As a result, the maps constructed from this North Dakota data are sparse. The maps constructed by Brown (1985) for the same three coals at similar O₂/coal ratios and coal feed rates, but an operating pressure of 1 atmosphere, have also been included in this analysis for purposes of comparison.

Carbon Conversion. Carbon conversion maps at 1, 5.5, and 10 atmospheres operating pressure, for the North Dakota, Wyoming, and Illinois No. 6 coals are shown in Figures 13-15, respectively. Figure 16 shows similar profiles obtained by Azuhata at 1 and 5 atm pressure, with Utah high volatile bituminous coal. The results for each coal, at all operating pressures, show several reaction regions within the gasifier. These regions, as discussed by Hedman, et al., (1982) include an intense flame zone in the fore-part of the reactor, where devolatilization and rapid conversion occurs, and a region of slow conversion in the lower 2/3 of the reactor where heterogeneous reactions occur. At atmospheric pressure, Brown (1985) observed approximately 75% carbon conversion at about 83 cm axial position. At both the elevated pressure levels, carbon conversions values of at least 90% were measured for all four coals at the same position. It is noted that the exit carbon conversion values for the Illinois No. 6 bituminous coal are only 83% and 89% respectively, yet conversions as high as 94% were measured at the 83 cm position in the reactor for these same two elevated pressure tests. A similar

Coal feed rate ~ 33 kg/hr
 O_2 /coal ratio (kg/kg) ~ 0.85
 Steam/coal ratio (kg/kg) = 0.0

Figure 13. Isocontours of carbon conversion (in percent) interpolated from local measurements for North Dakota lignite at three operating pressures.

Figure 14. Isocontours of carbon conversion (in percent) from local measurements for Wyoming subbituminous coal at three operating pressures.

Coal feed rate ~ 33 or 50 kg/hr
 O_2 /coal ratio (kg/kg) ~ 0.85
 Steam/coal ratio (kg/kg) = 0.0

Figure 15. Isocontours of carbon conversion (in percent) from local measurements for Illinois No. 6 bituminous coal at two operating pressure and two coal feed rates.

Figure 16. Isocontours of carbon conversion (in percent) interpolated from local measurements for Utah bituminous coal at two operating pressures.

result is also observed for the 5.5 atmosphere test of the North Dakota lignite. Only a fraction of the injected coal particles are dispersed away from the reactor centerline, and experience conversion in excess of 90%, while the average carbon conversion measured near the reactor exit may be lower.

Marked differences in carbon conversion among coals are observed in the elevated pressure maps. The carbon conversion of the lignite is essentially complete by the 22 cm. position, while significant reaction occurs between 22 and 83 cm. for the subbituminous and bituminous coals. The exit plane carbon conversion values for the lignite and subbituminous coal approach 100% while both bituminous coals show an 80% to 90% conversion.

Effects of pressure are also observed in the maps of carbon conversion. For all four coals, this effect is an acceleration of the observed conversion levels with increasing pressure. At high pressure, the reactions occur much closer to the inlet of the gasifier. A recirculation zone, marked by high local conversion values, is shown in the upper left hand corner of the atmospheric pressure maps. This zone has been observed by other investigators, including Hedman et al., (1982), Soelberg (1983) and Azuhata (1986a), but is not observed in any of the elevated pressure maps.

The effects of coal feed rate are indicated in the Illinois No. 6 bituminous coal maps, where operating pressure was held constant at 5.5 atmospheres while coal feed rate was increased from 33 to 50 kg/hr. A higher coal feed rate can have two effects which include: 1) an increased coal reaction rate resulting from the increased heat release rate and higher gasifier temperatures, and 2) decreased gasifier residence time. The increase in the exit carbon conversion value at the higher coal feed rate indicates that the increased coal reaction rate dominates over the decrease in residence time.

Gaseous Species Profiles. Carbon monoxide concentration contours, at each of the three pressure levels, are shown for each coal in Figures 17-19. Brown (1985) found in his atmospheric pressure tests that carbon monoxide forms rapidly in the intense flame zone, and reaches a maximum between the 60 and 80 cm. axial positions. The same type of behavior is observed in the elevated pressure maps, except that the maximum CO concentrations are often observed in the 22 cm. axial position. Carbon monoxide concentrations in the lower region of the reactor also show a dependence upon the operating pressure and coal feed rate. In the atmospheric pressure maps, CO concentrations decreased only slightly in the lower two thirds of the reactor. At 5.5 atmospheres pressure and a coal feed rate of 33 kg/hr, the carbon monoxide concentration decrease ranged anywhere from 2% to 16.5% in the same lower region of the reactor. No decrease in carbon monoxide concentration was observed in the lower two thirds of the reactor, in the 50 kg/hr test with Illinois No. 6 coal.

Brown (1985) showed in his atmospheric tests that carbon monoxide formation was strongly dependent upon coal volatile matter. "Higher amounts of volatile matter lead to higher heat release rates and hotter temperatures as the volatiles combust with oxygen. These higher temperatures lead to higher amounts of carbon monoxide in the gas phase through such reactions as the water-gas shift reaction". This same behavior is observed at elevated pressures. The tests with the Illinois No. 6 bituminous coal yielded the

Coal feed rate ~ 33 kg/hr
 O_2 /coal ratio (kg/kg) ~ 0.85
 Steam/coal ratio (kg/kg) = 0.0

Figure 17. Isocontours of mole % CO interpolated from local measurements for North Dakota lignite at three operating pressures.

Coal feed rate ~ 33 kg/hr
 O_2 /coal ratio (kg/kg) ~ 0.85
 Steam/coal ratio (kg/kg) = 0.0

Figure 18. Isocontours of mole % CO interpolated from local measurements for Wyoming subbituminous coal at three operating pressures.

Coal feed rate ~ 33 or 50 kg/hr
 O_2 /coal ratio (kg/kg) ~ 0.85
 Steam/coal ratio (kg/kg) = 0.0

Figure 19. Isocontours of mole % CO interpolated from local measurements for Illinois No. 6 bituminous coal at two operating pressures and two coal feed rates.

highest maximum and exit plane concentrations of CO, followed in decreasing order by the Wyoming coal and the North Dakota lignite.

CO₂ and H₂ concentration contours for the North Dakota lignite, Wyoming subbituminous and Illinois bituminous coals, at each of the three pressure levels are contained in Cope (1987). A definite effect of operating pressure on CO₂ and H₂ concentrations is not apparent from these tests. High concentrations of both species were measured in the upper regions of the gasifier, but these concentrations neither increased nor decreased in a regular manner as operating pressure was increased. An increase in the Illinois coal feed rate from 33 to 50 kg/hr, at constant pressure, had no definite impact on the measured concentrations of carbon dioxide and hydrogen.

Pollutant Formation-Utah Bituminous Coal

Nitrogen and sulfur pollutant formation data were collected toward the end of the previous gasification study (Hedman, et al., 1985) for Utah bituminous coal and in this study for the other three coals. Gasification results for the earlier work were reported by Azuhata, et al., (1986b). The pollutant formation results are summarized in the following sections of this report and in papers by Nichols, et al., (1987a), and (1987b).

Nitrogen Pollutants. One concern in coal conversion technology is the production of gaseous nitrogen pollutants. Coals contain about 0.5-2.0 weight percent of nitrogen, most of which is converted to volatile forms (N₂, NO, NH₃, HCN) in coal flames. The presence of nitrogen pollutants (NO, NH₃, HCN) in the gaseous product of a gasification process is undesirable. These pollutants can poison catalysts used for processes such as methanation (Axworthy, et al., 1976), or they are converted upon subsequent combustion primarily to NO which creates environmental concern or increases cleanup costs. Pollutant removal prior to use of the product gas also increases operating and equipment costs. It is of interest to understand how gasification process parameters can be adjusted to reduce the proportion of fuel-nitrogen which is converted to pollutant forms. This requires a detailed knowledge of the physical and chemical processes by which fuel-nitrogen is converted to gas phase species.

The findings from gasification studies reveal additional insight regarding nitrogen chemistry in coal flames beyond that obtained from combustion studies. Associated with the gasification environment are much higher temperatures in the primary reaction zone (due to use of oxygen rather than air as oxidant) and a higher degree of fuel-richness over-all than in combustion environments. Since during gasification, an appreciable portion of the fuel-nitrogen results in the fuel-rich products NH₃ and HCN, study of these intermediates is facilitated.

Numerous investigations into the fate of fuel-nitrogen during coal conversion have been conducted. Most of this work has been associated with combustion in air, and not gasification in oxygen. Price, et al. (1983) and Highsmith, et al. (1985) report work on nitrogen pollutants produced from entrained-coal gasification, but effects of pressure, flame structure and coal feed rate were not variables in these studies. Some nitrogen pollutant trends have been reported by Schlenger and Richter (1980) for the Texaco Coal Gasification Process, and by Hansen, et al. (1980) for high rate entrained-

coal gasification. Both of these studies were conducted at elevated pressures. However, only effluent data were reported and no comparison was made with similar gasification data at atmospheric pressure. Investigations of NO levels from pressurized, fluidized-bed combustion of coal have been reviewed and discussed by Chen, et al. (1981). Yields of fuel-NO from fuel-rich hydrocarbon flames at elevated pressure have been reported by Heberling and Boyd (1981). But, studies of pollutant formation at elevated pressure have not been extensive. Studies conducted on flame structure and coal feed rate effects during gasification have focused on carbon conversion and major gas species (Azuhata, et al., 1986a, 1986b).

The form of nitrogen in coal is thought to be primarily heterocyclic aromatic ring structures (Pohl and Sorifim, 1977; Malte and Rees, 1979), though this is difficult to ascertain, since removal of the nitrogen containing compounds from coal without their destruction is difficult. Independent of such a knowledge concerning the specific structural forms, a commonly proposed mechanism for fuel-nitrogen conversion (coal or otherwise) and reaction in the gas phase during high-temperature combustion is (Malte and Rees, 1979; DeSoete, 1975; Fenimore, 1979; Song, et al., 1981; Smith, et al. 1982; Glass and Wendt, 1982; Miller, et al. 1984; Morley, 1981):

This mechanism places the reactants into four main groups: a pool of HCN and CN, a pool of NH_i , and the two final products, N_2 and NO. Most of the fuel-nitrogen is thought to be converted early in the flame to the HCN, CN pool. The cyanide species decay to yield the second intermediate pool; N, NH, NH_2 , and NH_3 . The NH_i species are thought to be in partial equilibrium (Kaskan and Hughes, 1973) and are thought to form NO and N_2 through the competitive steps shown in Equation 1. A number of researchers have examined the kinetic details of the cyanide species decay to NO and N_2 and of the role which the NH_i species play as an intermediate in premixed and diffusion gaseous hydrocarbon flames. There are differing opinions as to the nature of the NH_i species, though there is general agreement that the homogeneous decay of NO is second order with respect to concentration. These kinetics have been extended to turbulent coal flames with encouraging success (Glass and Wendt, 1982; Hill, et al., 1984). Highsmith, et al. (1985) have also used Equation 1 to explain the fate of fuel-nitrogen during coal gasification. Equation 1 does not represent all the pathways investigated. Some others are the reduction of NO by char, the reaction of N_2 with hydrocarbon radicals, the conversion of NO to HCN and NH_i , and the production of thermal NO.

The extent to which the fuel-nitrogen was converted (nitrogen conversion) from the coal is shown in Figure 20 for the gasifier exit plane data. The conversion of a fuel-element to the gas phase was determined by measuring the elemental and ash content of the coal and of the collected char, with ash as

Figure 20. Extent of fuel-nitrogen release into the gas phase during gasification of Utah bituminous coal.

Figure 21. Extent of fuel-carbon release into the gas phase during gasification of Utah bituminous coal. (Symbols shown in preceding figure.)

an inert tracer. Of the variables considered, flame type (diffusion or premixed) had the largest effect on nitrogen conversion. The average nitrogen conversion was 83% for the diffusion flame and 92% for the premixed flame. Nitrogen conversion was slightly dependent on oxygen-coal mass ratio for the diffusion flame, but was not noticeably affected by pressure or by coal feed rate.

Carbon conversion values are shown in Figure 21. Conversion of carbon increased with oxygen-coal ratio, similar to the gasification data trends of various investigators reported by Smoot and Smith (1985) and by Azuhata, et al. (1986a). The premixed flame yielded significantly higher carbon conversion. This is in agreement with the findings of others (Smoot and Smith, 1985; Lewis, et al., 1982). As found earlier (Azuhata, et al., 1986b), it was not evident that carbon conversion was substantially affected by increasing pressure, up to 10 atm. The extent of nitrogen conversion exceeded that of carbon conversion. For the diffusion flame injector, the average carbon conversion was 51% compared to 83% already mentioned for nitrogen. A similar trend was observed by Highsmith, et al. (1985) during gasification. Malte and Rees (1979) reported the ratio of nitrogen-to-carbon converted to be between 1.3 and 2.0 for coal gasification. Of course, this ratio must approach unity as carbon conversion approaches 100%.

Though nitrogen conversion showed some dependence on flame type and oxygen-coal mass ratio, it showed a lesser magnitude of dependence on these variables than carbon conversion showed. This may be because the nitrogen conversion values are high. In general, as nitrogen conversion approaches 100%, there must be less dependence on process variables. A possible explanation for high nitrogen conversion is the behavior of nitrogen conversion with temperature. Carefully controlled coal pyrolysis experiments (Pohl and Sarofim, 1977; Blair, et al., 1977) have shown that nitrogen evolution is more sensitive to temperature than total mass evolution. For the gasifier of this study, gas residence times within the gasifier varied from approximately 200 ms to 2.2 s, depending on pressure and feed rates. Peak local temperatures in the gasifier were predicted to be near 3150 K using the generalized two-dimensional pulverized coal gasification model (PCGC-2) (Boardman, 1987). Thermodynamic calculations predicted peak local adiabatic flame temperatures of near 3200 K. It appears that sufficient temperatures existed in the gasifier for a sufficient length of time such that nitrogen conversion approached completion. At this point it was relatively insensitive to temperature changes which resulted from changing operating parameters.

The exit char measurements indicated only the total nitrogen converted, and did not distinguish between the fuel nitrogen converted during devolatilization and char oxidation. However, it has been shown (Azuhata, et al., 1986b; Soelberg, et al., 1985; Brown, 1985) during entrained-coal gasification, that the majority of the coal mass loss occurs very early in the flame, probably during devolatilization. Since nitrogen conversion exceeds carbon conversion, the nitrogen conversion would also exceed total coal mass loss. This suggests that the great majority of the nitrogen was converted during devolatilization.

Figure 22 shows measured NO, NH₃, and HCN concentrations near the gasifier exit for all conditions examined. From a nitrogen balance, it is estimated that over one-half of the converted fuel-nitrogen was converted to

Figure 22. Observed effects of pressure, oxygen-coal mass ratio, coal feed-rate, and flame structure on gas-phase nitrogen pollutant species during gasification of Utah bituminous coal. (Symbols defined in Figure 20.)

N₂. Large amounts of NH₃ and HCN were produced, while the fraction of fuel nitrogen converted to NO was small. Peck, et al. (1984) reported that about 45% of the fuel-nitrogen evolved as N₂ from fuel-rich combustion of pulverized coal. Highsmith, et al. (1985) estimated that N₂ was the major product formed from the fuel-nitrogen at atmospheric pressure.

As seen in Figure 22, pressure had a dramatic effect on exit NO levels. At atmospheric pressure, the NO levels increased with increasing oxygen-coal ratio from approximately 30 to 300 ppm. These data compare well to the gasification data of Price, et al. (1983) and Highsmith, et al. (1985) who measured NO levels at atmospheric pressure in the range of 70 to 400 ppm from the effluent of entrained-flow gasification of Utah bituminous coal. However, exit NO levels at 4.9 atm and 10.4 atm were near zero (less than 10 ppm) for all coal feed rates, oxygen-coal ratios and for both flame types. Chen, et al. (1981) reviewed the NO data from previous investigations of fluidized-bed coal combustion at elevated pressures. These data also showed that NO decreased significantly as pressure was increased. They attributed this decrease to increased residence time and enhanced NO decay kinetics. Heberling and Boyd (1981) observed the yield of NO from fuel-nitrogen in laminar diffusion flames to decrease sharply when the pressure was increased. With a fuel composed of CH₄/H₂/CH₃/NH₂, the NO dropped by a factor of 9 as pressure was increased from 1 to 16 atm. Heberling and Boyd (1981) concluded that there was a decrease in the amount of fuel NO produced near the flame front. This decrease in NO will be discussed further in the sub-section on profile data.

NH₃ and HCN levels decreased with increasing oxygen-coal ratio, as expected for these fuel-rich species. For the diffusion flame, NH₃ levels approximately doubled while HCN levels decreased by the same factor as pressure increased from 1 to 10.4 atm. Hansen, et al. (1980) also observed HCN to decrease as pressure was increased from 6 to 11 atm using a gasification diffusion flame. Within the accuracy of the data, it appears that the amount of fuel-nitrogen converted to N₂ was not affected by increasing pressure.

The premixed flame produced lower levels of NH₃ and HCN and thereby higher levels of N₂ than did the diffusion flame. This may be due to higher temperatures in the premixed flame though no conclusive evidence was found to verify that the premixed flame was necessarily hotter. Peck, et al. (1984) noted a decrease in NH₃ and HCN at higher flame temperatures.

The effect of coal feed rate on NH₃ and HCN production was not large, though NH₃ levels at the higher coal feed rate were somewhat lower for the premixed flame. Possibly, the higher coal feed rate resulted in greater volumetric heat conversion rate, while heat loss through the reactor walls would not have been significantly changed. Thus, the overall fraction of heat loss was reduced at the higher coal feed rate, yielding higher average temperatures. This increased temperature could have been the cause of lower NH₃ levels. However, any increase in temperature caused by increased coal feed rate could not have been large, as Figure 21 shows that coal feed rate had no effect on carbon conversion.

Profile data were obtained at an oxygen-coal ratio of 0.90, a pressure of 4.9 atm, and a coal feed rate of 35 kg/h, using the premixed flame, and

results compared to profile data previously obtained at 1 atm pressure (Highsmith, et al., 1985). The gasifier used for acquisition of the atmospheric data was of shorter length, but otherwise the same as in this study. Samples were collected at several radial locations between the centerline and the wall for each of several axial locations ranging as close as 6 cm aft of the injection point to near the gasifier exit.

Contours of NO concentration data are shown in Figure 23, for both pressures. Lines were constructed by the interpolation of the discrete data points collected, and are therefore of a qualitative nature. As noted previously (Hedman, et al., 1982; Highsmith, et al., 1985; Soelberg, et al., 1985), three distinct reaction zones exist: an intense reaction (flame) core with large concentration gradients, surrounded by a recirculation zone near the reactor walls, and followed downstream by a less intense zone of lesser concentration gradients. The intense flame core is reduced in size for the 4.9 atm case, as would be expected with increased pressure at constant mass feed rates.

At 4.9 atm, the maximum measured NO level was 3300 ppm at the centerline, 6 cm aft of the injector. The levels decreased from there to near zero within 80 cm aft of the injector. The atmospheric NO map shows a similar decrease, but further reveals an increase and a maximum NO value. It was presumed that in the 4.9 atm case, the NO also increased to some maximum, and then decreased after the oxygen supply became depleted. Only the decrease was measured, and the increase evidently occurred prior to the 6 cm axial sampling location. The high NO levels near the injector for both maps are due to the abundance of oxygen present there. As the fuel-nitrogen was converted in an oxygen containing environment, the HCN pool was rapidly converted to NO.

As discussed in the previous section, the exit NO levels at 4.9 atm were near zero compared to several hundred ppm NO at 1 atm pressure for both flame types. The profile data using the premixed flame reveal that at 4.9 atm pressure, the peak NO levels were higher than at 1 atm. Clearly, increased pressure did not decrease the peak amount of NO produced near the flame. However, the 4.9 atm data show substantially greater post-flame decay, compared to the decay at atmospheric pressure.

The question arises as to what extent this increased NO decay was due to higher pressure, or to increased residence time. The increased residence time resulted from increasing gasifier pressure while maintaining constant mass feed rates. Gas residence time values were calculated from averaged gas velocities as a function of axial distance for both the 4.9 atm and the atmospheric cases. The gas velocities were determined using a generalized computer model (Smoot and Smith, 1985). Figure 24 shows centerline NO measurements as a function of residence time. Also included in Figure 24 for comparison are independent data from fuel-rich ($SR = 0.4, 0.6$) combustion of Utah bituminous coal at atmospheric pressure (Glass and Wendt, 1982; Dannecker and Wendt, 1984). Apparently, both residence time and pressure play important roles in increasing the extent of NO decay. Heterogeneous decay of NO was considered negligible in the gasifier, based on the findings of Glass and Wendt (1982) for fuel-rich flames.

An additional set of gasifier tests were performed for the purpose of independently distinguishing between the effects of residence time and

a) Atmospheric Pressure
(Highsmith, et al. 1985)

b) 4.9 atm
(Nichols 1985)

Figure 23. Nitric oxide concentration contours measured during gasification of Utah bituminous coal: 1.0 atm, top; 4.9 atm, bottom; NO concentrations are reported as dry inert-free ppmv.

pressure. NO measurements were made at the gasifier exit at differing pressures while residence time was maintained approximately constant. Measurements were also made at differing residence times while pressure was held constant. The residence time was varied by varying the coal feed rate. The resulting NO measurements are shown in Figure 25. The residence time values were determined as previously described by assuming a linear temperature profile in the gasifier.

Increasing pressure by only one atmosphere had a dramatic effect on the NO levels while changing residence time had little effect. This latter observation is in disagreement with observations made regarding Figure 24. This may be the result of changing heat loss (and temperature) patterns among various coal feed rates. Concentrations of NO are expected to be highly sensitive to temperature. Thus it appears that pressure plays the dominant role in decreasing the NO levels.

The Total Fixed Nitrogen (TFN) is defined to be the sum of the NH_3 , HCN, and NO levels. As also seen in Figure 25, increased residence time decreased TFN levels, particularly at 1 atm. It is not evident that pressure alone had a significant effect on TFN levels. A strong interaction existed between the two effects.

Values of nitrogen conversion and carbon conversion are shown in Figure 26. Nitrogen conversion was not affected significantly by residence time or pressure. Nitrogen conversion exceeded carbon conversion which is consistent with the previous observations.

As discussed previously, the dominant mechanism for NO decay is generally thought to be of the form

$$-d[\text{NO}]/dt = k[\text{NO}] [I] \quad (2)$$

where I represents a nitrogen-containing intermediate, though the nature of this intermediate is subject to various opinions. Dividing both sides of Equation 2 by [NO] and assuming ideal gas, the semi-logarithmic slopes in Figure 24 are theoretically:

$$-d(\log[\text{NO}])/dt = k y_i P / (RT) \quad (3)$$

where y_i is the mole fraction of the intermediate, and P and T are pressure and temperature. Thus, the decay rate of the logarithm of NO concentration is expected to increase approximately in proportion to pressure. From the experimental data of Figure 24, it is clear that the NO decay rate is greater at 4.9 atm. This supports the theory discussed above and indicates that pressure is important during NO decay, because it increases the rate of NO decay.

Conclusions. For these gasification tests with Utah bituminous coal, fuel-nitrogen conversion from the coal showed little dependence on oxygen-coal mass ratio, pressure, or coal feed rate, but showed some dependence on flame

Figure 24. Influence of residence time on extent of NO decay, and influence of pressure on NO decay rate for gasification and combustion of Utah bituminous coal. (All values shown are centerline measurements.) (SR=0.60: Dannecker and Wendt, 1984, SR=0.40: Glass and Wendt, 1982).

Figure 25. Effects of pressure and residence time on gasifier effluent nitrogen species concentrations. a) NO b) TFN (sum of NH_3 , HCN and NO).

Figure 26. Effects of pressure and residence time on gasifier carbon and nitrogen conversions.

type; the premixed flame gave 92% nitrogen conversion compared to 83% for the diffusion flame. The extent of fuel-nitrogen conversion was greater than the extent of fuel-carbon conversion. The reason for the high nitrogen conversion for all conditions tested, was suggested to be the high flame temperatures (over 3000 K) characteristic of gasification in oxygen. Evidence was provided that most of the fuel-nitrogen was converted during devolatilization, and not during char oxidation.

The fate of the nitrogen after being converted from the coal was found to be influenced by coal feed rate. Material balance analyses indicated that the majority of the converted fuel-nitrogen was converted to N_2 . Appreciable quantities of NH_3 and HCN were measured in the effluent, with smaller quantities of NO. For the diffusion flame at 10.4 atm, the exit levels of NH_3 produced were approximately double those produced at atmospheric pressure, while the HCN levels at 10.4 atm were approximately half those at atmospheric pressure. Exit N_2 levels were not significantly affected by pressure. The premixed flame yielded lower exit levels of NH_3 and HCN than the diffusion flame.

The 4.9 and 10.4 atm data showed dramatically reduced effluent NO concentrations compared to atmospheric pressure values. It was shown that the reduction in effluent NO was due to increased rate of NO decay at higher pressure, and possibly to a lesser extent, increased residence times. The peak NO levels produced early in the gasifier flame were not decreased by increased pressure. This agrees with postulated theories that NO decay rate is second order with respect to gas species concentration.

Sulfur Pollutants. One concern in coal combustion processes is the production of gaseous sulfur pollutants. Sulfur oxides emissions from combustion of coal are a major contributor to acid rain. These sulfur gases can be removed by scrubbing, but scrubbing requires significant equipment costs. The injection of sorbents has been investigated because of the low cost and wide availability of metal oxides for sorbent material (Kramlich, et al., 1986). Studies have focused on improving the utilization of the sorbent. Little or no study has been made to examine the effects of combustion chamber pressure on sorbent reactivity and sorbent utilization. The fuel rich environment in a coal gasifier is heavily laden with char particles. Understanding the interaction of char with sulfur gas species in high-pressure gasification may provide insight as to how pressure could be used to enhance sulfur capture by solid particles.

Sulfur conversion is the percent of fuel sulfur which escaped from the solid coal and resulted in gas phase sulfur species. Sulfur conversion values for the atmospheric and 10.4 atm tests are shown in Figure 27. These sulfur conversion values were determined from the gas phase sulfur species measurements using carbon as a tie element. The 4.9 atm sulfur conversion data are not included, because the SO_2 measurements at this pressure were not available.

From Figure 27, the sulfur conversion decreased about 15% as pressure increased from atmospheric to 10.4 atm. This effect of pressure on sulfur conversion was not dependent on oxygen-to-coal mass ratio. The reason for lower sulfur conversion at higher pressure may be the retention of sulfur by char. It is known (Attar, 1977; Attar and Messenger, 1983) that reactions of

Figure 27. Sulfur and carbon conversion measured in gasifier effluent samples carbon conversion data reported by Nichols, et al. 1987 and Azuhata, et al. 1986.

Figure 28. Distribution of gas phase sulfur, as measured in gasifier effluent.

basic minerals with H_2S are one of the major reasons for the retention of sulfur in char. Trapping of sulfur in the form of stable heterocyclic organic compounds is also believed to account for the retention of sulfur in char. Attar (1977) indicates that trapping of sulfur by the back reaction of H_2S with various organic groups is thermodynamically favorable.

At high pressure, the flame zone was smaller, and residence time was larger. Gas residence time is approximately proportional to pressure. This increase in residence time could have provided increased opportunity for reactions to occur where sulfur was captured by char. The increased pressure could also have enhanced the mechanism of sulfur capture by the char. Measurements of the composition of the gasification char samples also show the increased sulfur capture by the char. The amount of sulfur found in the char samples was higher than was expected based on the amount of sulfur measured in the gas phase. Previous space resolved gasification measurements (Highsmith, et al., 1985) showed that sulfur conversion reached a peak near the flame zone, and then decreased to a lower-than-peak level at the gasifier exit. These data indicated that sulfur capture by the char might be occurring in a gasifier. The conversion data of Figure 27 suggest that increasing gasifier pressure increased the effectiveness of this sulfur capture by char.

Sulfur conversion increased with increasing oxygen-to-coal mass ratio. This was expected, based on previously reported gasification data (Smoot and Smith, 1985) which show coal mass release to be strongly dependent on oxygen-to-coal mass ratio. Sulfur conversion was expected to be correlated with coal mass release. Figure 27 includes carbon conversion values (based on ash balance). Carbon conversion values for both atmospheric and 10.4 atm pressures are similar to sulfur conversion values at 10.4 atm pressure. Sulfur conversion at atmospheric pressure exceeds carbon conversion. It has been shown earlier (Azuhata et al., 1986b; Nichols et al., 1987a) that carbon conversion was not affected by increasing pressure up to 10.4 atm.

Figure 28 shows the distribution of the gas phase sulfur, which converted from the coal. The majority of the converted sulfur resulted in H_2S at both atmospheric and 10.4 atm pressures. At atmospheric pressure, 50-60% of the converted sulfur resulted in H_2S , with 20-35% resulting in SO_2 , 10-13% resulting in CS_2 , and 6-8% resulting in COS . The ratio of SO_2 to H_2S increased from 0.3 to 0.8 as oxygen-to-coal mass ratio increased from 0.67 to 1.08. At 10.4 atm pressure, 85-90% of the converted sulfur resulted in H_2S , with 6-8% resulting in SO_2 and 6-8% resulting in COS . No CS_2 was detectable at 10.4 atm pressure. Thus, a shift in the distribution of gas phase sulfur was seen. Increasing pressure increased the relative proportion of H_2S , while decreasing the sum of the remaining sulfur species.

Equilibrium calculations (Nichols, 1985) predict that pressure has no noticeable effect on the sulfur species distribution (gas phase) during a combustion process. Sulfur species in combustion systems have been noted to be near equilibrium (Kramlich et al., 1981; Fenimore and Jones, 1965). If sulfur reactions in a coal gasifier are approximated well by equilibrium, then the distribution of SO_2 and H_2S near the flame should not have changed with pressure. Vogel et al. (1974) observed during fluidized-bed combustion of coal that SO_2 concentration was relatively unaffected by changes in system pressure between 1 and 8 atm. The gasification environment was more fuel rich, and more particle-laden than the combustion environment. This again

leads to the conclusion that interactions of sulfur species (particularly H_2S) with char are responsible for the changes in the fate of fuel-sulfur with changing pressure.

The measured concentrations (ppm, dry basis) of H_2S , SO_2 , COS and CS_2 are shown in Figure 29. Levels of H_2S were higher at 4.9 atm than H_2S levels at atmospheric pressure. This reflects the observation in Figure 28, that higher pressure shifted the distribution of gas phase sulfur towards H_2S . Levels of H_2S at 10.4 atm exhibited a different trend. This may be a result of two competing effects. As pressure increased, the fraction of converted sulfur resulting in H_2S increased, thus tending to increase H_2S . But, as pressure increased, sulfur conversion decreased, tending to decrease H_2S . The net effect of these two is difficult to resolve, since the sulfur conversion values at 4.9 atm pressure are not available.

Levels of SO_2 decreased markedly with increasing pressure. In previously reported nitrogen species measurements (Nichols et al., 1987a), a similar trend was observed for NO levels. It was shown that NO levels reached a peak near the flame, after which they decayed to the level measured in the effluent gases. It was shown that the magnitude of this peak NO level was not affected by pressure between atmospheric and 4.9 atm, but the extent of post flame NO decay was increased by the higher pressure. The behavior of the SO_2 may be analogous to the behavior of the NO . Thus, the observed decrease in effluent SO_2 was attributed to enhanced rate of SO_2 decay, and increased residence time, both of which resulted from increasing the gasification pressure. The redistribution effect shown in Figure 29 indicates that SO_2 decayed to H_2S .

The CS_2 levels also decreased markedly with increasing pressure. Levels of near 150 ppm CS_2 at atmospheric pressure compare to no detectable CS_2 at 10.4 atm pressure. The sensitivity limit of the gas chromatograph and flame photometric detector used to measure CS_2 was near 10 ppm CS_2 . Levels of COS were only slightly affected by pressure. Levels of COS increased slightly as pressure increased from atmospheric to 4.9 atm. At 10.4 atm pressure, levels of COS decreased to below what they were at atmospheric pressure. This may be a result of competing effects, as discussed with relation to the observed H_2S concentrations. Both CS_2 and COS were affected by oxygen-to-coal mass ratio, at all levels of pressure. Increased oxygen-to-coal mass ratio tended to increase COS and decrease CS_2 .

Measurements were made of the sulfur retained in char, and of the gas phase sulfur species formed during entrained-flow gasification of a Utah bituminous coal. The sulfur conversion decreased approximately 15% as gasification chamber pressure increased from atmospheric to 10.4 atm pressure. There appears to be significant sulfur capture by the char occurring. Sulfur conversion increased with increasing oxygen-to-coal mass ratio. Sulfur conversion was greater than carbon conversion at atmospheric pressure. The distribution of gas phase sulfur changed with changing pressure. The relative proportions of SO_2 and CS_2 decreased while the proportion of H_2S increased. This was not predicted by equilibrium calculations, nor was it observed in leaner combustion environments. The high degree of fuel richness, and sulfur gas-char interaction were reasoned to be responsible for this gas phase redistribution with changing pressure. It was observed that as oxygen-to-coal mass ratio increased levels of H_2S and CS_2 decreased, while levels of SO_2 and COS increased.

Figure 29. Sulfur species concentrations in gasifier effluent.
a) H_2S b) SO_2 c) COS d) CS_2

Pollutant Formation for Other Coals

Test Conditions. The sulfur and nitrogen pollutant data obtained for the parametric variation and mapping tests with the three additional coal types at elevated pressure are reported in detail in Appendices A and B. Key observations from parametric variation tests are summarized below. Further analysis of the parametric variation tests and mapping tests is reported in the M.S. thesis by Smith (1987).

Two pressures (5.5 and 10 atm), two O_2 /coal ratios (0.7 and 0.85 kg O_2 /kg coal), and two coal feed rates (33 and 50 kg/hr) were investigated. An injector that premixed the coal and oxygen streams was used. The coals were pulverized to about 50 μ m mass mean diameter to eliminate particle size as a variable (see Figure 6). Results were obtained for the North Dakota, Wyoming and Illinois coals (see Table 2). Sulfur (0.3-4%) and moisture (11-34%) percentages varied significantly among coals while nitrogen variation was less (0.5-1.1%).

Nitrogen Pollutants. The amount of nitrogen in the parent coal did not influence the amount of nitrogen converted to the gaseous nitrogen species. The nitrogen conversion generally exceeded 90% (See Appendix A). No measurable nitric oxide (NO) was observed at the gasifier exit in any of these tests at elevated pressure. Figures 30 and 31 summarize the effect of O_2 /coal ratio and coal rank on the level of NH_3 and HCN pollutants respectively at operating pressures of 5.5 and 10 atm pressure. The Wyoming subbituminous coal, with 0.6% fuel-N produced the highest concentration of NH_3 . The Illinois No. 6 bituminous coal with 1.1% fuel-N produced the least amount of NH_3 . Conversely, the bituminous coal produced the greatest amount of HCN and the subbituminous coal the least. Table 6 compares the relative distribution of converted fuel nitrogen among the nitrogen pollutant species.

TABLE 6

PERCENT OF CONVERTED FUEL NITROGEN
(O_2 /coal = 0.7, Pressure = 5.5/10.0 atm.)

<u>Coal Rank</u>	<u>HCN</u>	<u>NH_3</u>	<u>NO</u>
Bituminous	86/78	14/22	<<1/<<1
Subbituminous	11/11	89/89	<<1/<<1
Lignite	36/30	64/70	<<1/<<1

At atmospheric pressure, Brown (1985) showed that the relative distribution of converted fuel-N for each coal was similar with the exception that NO was significant (2-16%). The relative amounts of HCN and NH_3 produced by the Utah bituminous coal appeared to resemble the results of the Wyoming coal.

Sulfur Pollutants. The measured sulfur pollutant species were hydrogen sulfide (H_2S), carbonyl sulfide (COS), carbon disulfide (CS_2), and sulfur dioxide (SO_2). Figure 32 summarizes the effect of O_2 /coal ratio and coal rank on the levels of H_2S measured for the two elevated operating pressures.

Figure 30. Concentration of ammonia at the exit plane (Dry basis).

Figure 31. Concentration of hydrogen cyanide at the exit plane (Dry basis).

Hydrogen sulfide (H_2S) was the dominant sulfur species in the gas phase during gasification. This has been observed by other investigators as well (Nichols, 1987b). The amount of H_2S measured in the gasification products corresponded directly with the amount of sulfur in the parent coal. An increase in pressure had little effect on the level of H_2S formed as shown in Figure 32.

Figure 33 shows the effect of O_2 /coal ratio and coal rank on COS concentration at the two operating pressures. Carbonyl sulfide was the second most abundant sulfur species found in the gas phase. COS concentrations also varied with the amount of sulfur in the parent coals. Throughout the parametric variation tests there was no detectable carbonyl sulfide (CS_2) or sulfur dioxide (SO_2) in the gas phase. Other investigators have also observed this during gasification at elevated pressures.

With the exception of the Illinois coal, Brown (1985), showed that H_2S accounted for 90-95% of the converted sulfur at the reactor exit, for the North Dakota, Wyoming and Utah coals at atmospheric pressure. The Illinois coal produced relatively large amounts of all sulfur gas species (H_2S , COS, CS_2 and SO_2), H_2S again being dominant. The results of Brown (1985) and this current study show that the effluent concentrations of CS_2 and SO_2 decrease with pressure.

Subtask 1.2 - Injector Characterization

Objectives and Injector Design

The objectives of this subtask were threefold. First, a comprehensive gasification model (PCGC-2) was to be used to design and evaluate four gasifier injectors for various O_2 /coal and steam/coal ratios and reactor chamber pressures. Second, the performance of each injector was to be experimentally determined during entrained coal gasification tests for a series of test variables. Results were to be compared to model predictions. The third objective was to provide experimental mapping data that could be used for interpretation of test results and for further code development. The experimental work focused on Injectors B, C, and D. Experimental mapping data, and to some extent, optimization data, were already available for Injector A from previous laboratory work (Hedman, et al., 1985; Azuhata, et al., 1985b).

Figure 34 illustrates four different injectors investigated. Injector A, the premixed injector, and Injector B, the parallel stream diffusion injector, are injectors that have been studied in the past at this laboratory (Azuhata et al., 1986b). Injector C, the swirled primary stream diffusion injector, and Injector D, the impinging secondary stream diffusion injector, were not previously studied at this laboratory.

Coal Properties

The coal used in the injector characterization study for both the experimental phase and PCGC-2 modeling phase was a Utah Bituminous coal from the Valley Camp mine in Central Utah. A Utah bituminous coal was chosen so that the results of this study could easily be compared to past studies done at BYU with Injector A (Hedman, et al., 1985). Ultimate, proximate and

Figure 32. Concentration of hydrogen sulfide at the exit plane (Dry basis).

Figure 33. Concentration of carbonyl sulfide at the exit plane (Dry basis).

Figure 34. Schematic diagram of the four injectors.

mineral analyses and particle size distribution are shown in Table 7. The mass mean particle size of the coal was 48 microns.

Test Program

Table 8 summarizes the reactor operating conditions and the experimental tests. A complete data summary is found in Appendix C. The coal feed rates, reactor pressure, O₂/coal ratios and steam/coal ratios shown in Table 8 for the mapping tests are the average values from the mapping tests. The mapping tests for Injector C were initially started at 5.5 atm. Problems with burnup of the injector tip necessitated the map be done at 1.0 atm.

Data Reliability

Air Contamination. Gas samples that were taken throughout the test program were suspected of having various degrees of air contamination diluting the sample. Measureable amounts of molecular oxygen were not expected at the reaction chamber exit plane because of the very low stoichiometric ratios (< 0.5 for O₂/coal ratios 1.0 and smaller), but O₂ was observed. With air dilution, the ratio leaving excess N₂ to oxygen leaving would be the same as that in air, 3.76. In order to check for air dilution in the gas samples, mass balance closures on elemental nitrogen were performed. All of the excess N was assumed to be molecular N₂. A molar flow rate of excess N₂ was computed and compared to the molar flow rate of molecular oxygen leaving the gasifier. Figure 35 summarizes this relationship for all three Injectors, B, C, and D. Figure 35 suggests a linear relationship between the measured molecular O₂ and the computed excess N₂ exiting the gasifier. The line plotted on Figure 35 has a slope of 3.76 and an intercept of 0, and represents the expected linear relationship for air contamination in the gas samples. The plotted data do suggest that air contamination was responsible for the O₂ found in the gas samples taken at the gasifier exit plane. As postulated the samples that had good nitrogen balance closures had no measureable molecular oxygen. Consequently, all of the optimization data points were corrected by adjusting the measured values of N₂ until the elemental nitrogen balance showed no excess N₂ was present and the mole fraction of molecular oxygen was set equal to zero. The argon concentrations were also adjusted assuming the N₂ and O₂ removed represented air contamination.

Modified Local Mass Balances. The estimation of gas phase parameters (n, q, f) from gas phase measurements using Equation 3 and overall coal conversion from particle phase measurements (assuming ash could be used as a solid phase tracer) allowed for evaluation of particle-gas phase agreement using Equation 4.

$$\frac{\dot{m}_{\text{gas}}^{\text{in}}}{(1-n)} = \dot{m}_{\text{coal}}^{\text{in}} \times C_{\text{coal}} + \dot{m}_{\text{gas}}^{\text{in}} \quad (4)$$

where $\dot{m}_{\text{gas}}^{\text{in}}$ = total mass flow rate of gas entering the gasifier
 $\dot{m}_{\text{coal}}^{\text{in}}$ = total mass flow rate of coal entering the gasifier
 C_{coal} = coal conversion (predicted from char)
 n = coal gas mixture fraction (predicted from gas, see Equation D-1 and discussion in Appendix D)

TABLE 7

PHYSICAL AND CHEMICAL PROPERTIES OF THE UTAH BITUMINOUS COAL

<u>Elemental Analysis</u> (% Dry Basis)		<u>Proximate Analysis</u> (% Dry Basis)	
Ash	8.6	Ash	8.56
Carbon	71.8	Volatile	43.2
Hydrogen	5.0	Fixed Carbon	48.3
Nitrogen	1.6		
Sulfur	0.4	Btu/lb (dry)	12900
Oxygen	12.5	% Moisture	2.4

<u>Mineral Analysis</u>	<u>wt. %</u>	<u>Ash Fusion Temp (K)</u>	<u>Reducing</u>
Silicon Dioxide	59.4	Initial	2225
Aluminum Dioxide	17.0	Softening	2288
Iron Oxide	3.7	Hemispherical	2361
Calcium Oxide	8.7	Fluid	2435
Magnesium Oxide	2.1		
Sodium Oxide	1.1	Silicon/Aluminum Ratio	3.50
Potassium Oxide	0.7	Iron/Calcium Ratio	0.43
Titanium Dioxide	1.3	Base/Acid Ratio	0.21
Phosphorus Pentoxide	0.6	Sulfur Trioxide	5.03

<u>Particle Size Distribution</u>			
<u>Range (μm)</u>	<u>wt. %</u>	<u>Range (μm)</u>	<u>wt. %</u>
0.0 - 8.0	1.43	32.0 - 40.3	11.18
8.0 - 10.1	2.72	40.3 - 50.8	13.36
10.1 - 12.7	3.46	50.8 - 64.0	13.81
12.7 - 16.0	4.30	64.0 - 80.6	12.39
16.0 - 20.2	6.04	80.6 - 101.6	8.19
20.2 - 25.4	7.84	101.6 - 128.0	4.53
25.4 - 32.0	9.88	128.0 - 161.0	0.87

TABLE 8

SUMMARY OF EXPERIMENTAL TEST CONDITIONS AND SAMPLES TAKEN IN THE
INJECTOR CHARACTERIZATION WORK

<u>Test Series</u>	<u>Total Samples Collected</u>	<u>Coal Feed Rate (kg/hr)</u>	<u>Reactor Pressure (atm.)</u>	<u>O₂/Coal Ratio</u>	<u>Steam/Coal Ratio</u>
checkout (Injector A)	44	33	1.1-5.5	0.6-1.2	0.0
<u>Utah coal (diffusion flame, parallel stream injection, Injector B)</u>					
optimization	30	25-40	1.1-5.8	0.6-1.4	0.0-0.3
mapping	23	33	5.5	0.85	0.0
<u>Utah coal (diffusion flame, swirled primary, Injector C)</u>					
optimization	25	26-48	1.1-5.6	0.6-1.0	0.0-0.4
mapping	5	27	5.4	1.09	0.0
mapping	22	34	1.2	0.84	0.0
<u>Utah coal (diffusion flame, impinging secondary, Injector D)</u>					
optimization	21	25-46	1.1-5.8	0.7-1.3	0.0-0.3
mapping	20	34	5.4	0.84	0.0

Figure 35. A scatter plot of the molar flow rate of excess N_2 leaving the gasifier determined from elemental N mass balances related to the molar flow of molecular O_2 leaving the gasifier. The solid line represents the molar ratio of O_2 to N_2 in air.

Equation D-2 (discussed in Appendix D) estimates of η were found to be consistently larger than values of η that would satisfy Equation 4 (Sowa, 1987). This result was not surprising since Equation D-2 was derived assuming that every element in coal converts to the gas phase at the overall coal conversion rate (Smoot and Smith, 1985). Since coal H, N, and O were found to convert at faster rate than coal over the entire range of coal conversions measured, a positive biasing of η was given in Equation D-2 by assuming these elements converted at the same rate as coal (Sowa, 1987). The positive biasing of η was removed when Equation D-2 was modified by adding an elemental conversion scaling factor to the term containing η resulting in Equation 5.

$$w_i^g = \eta \frac{C_i}{C_{\text{coal}}} w_i^{\text{coal}} + \gamma w_i^w + f w_i^p + (1 - \eta - \gamma - f) w_i^s \quad (5)$$

where C_i = conversion of element "i" to the gas phase (predicted from particle phase)
 C_{coal} = conversion of coal (predicted from particle phase)

In conclusion, all of the optimization data for the injector characterization work reported herein used the modified local mass balance, Equation 5 to predict the local water mole fractions and the gas phase parameters (η , q , f). Further discussion of the differences in the estimating of H_2O , η , γ , and f through the use of Equation D-3 and Equation 5 can be found in Sowa (1987).

Mass Balance Closures. During the optimization tests, data reliability was checked by computing the overall mass balance closures. In order to compute mass balance closures, a flat mass flux profile and completely mixed conditions were assumed for each exit plane measurement. Table 9 shows the results of the overall mass balance closures for Injectors B, C, and D.

Effects of Operating Variables

Effects of O_2/coal ratio (0.7-1.0), steam/coal ratio (0.0-0.3) and pressure (1.0-5.5 atm) were investigated. A Box-Behnken statistical design was used. Additional independent variables were argon carrier gas feed rate, window purge feed rate, coal feed rate and reactor chamber heat loss. The values for all of the independent variables are reported in Appendix C. These additional variables were present due to mechanical constraints of operating the gasifier. No attempt was made to quantify the effect of argon carrier gas feed rate and window purge feed rate on the process performance.

General Trends. Identification of significant independent variables (O_2/coal , pressure, steam/coal, injector-type, heat loss and interactions) was performed for several dependent variables (Y_{CO} , Y_{CO_2} , Y_{CH_4} , Y_{H_2O} , C_C , C_H , C_N , C_{coal} , cold gas efficiency, and exit gas temperature) using a statistical analysis of covariance model. Three levels of significance were defined: definite, probable, possible. Definite significance implies that a given independent variable was found to significantly effect a given dependent variable in every statistical model examined. Probable significance implies at least 75% of the statistical models considered showed a significant relationship between an independent and dependent variable. Possible significance implies at least 50% of the statistical models considered showed

TABLE 9

SUMMARY OF THE MASS BALANCE CLOSURES AND PROPAGATION OF ERRORS
TECHNIQUE FOR INJECTORS B, C, AND D

<u>Mass Balance</u>	Average Closure Values Injector Type			Standard Deviations Injector Type		
	<u>B</u>	<u>C</u>	<u>D</u>	<u>B</u>	<u>C</u>	<u>D</u>
C	1.02	1.02	1.02	0.01	0.04	0.03
H	0.96	1.00	1.06	0.10	0.12	0.16
O	0.97	0.98	0.98	0.02	0.05	0.03
N	1.00	1.00	1.00	0.00	0.00	0.00
S	1.73	1.37	1.56	0.98	0.22	0.51
Ar	1.12	1.15	1.14	0.27	0.30	0.23
Overall	0.99	1.01	1.03	0.04	0.06	0.06

a significant relationship between an independent variable and a dependent variable. An explanation of the statistical models that were considered is available in Sowa (1987). Table 10 summarizes which independent variables showed significant relationships to specific dependent variables. These results apply only for the ranges of O_2 /coal, pressure and steam/coal investigated experimentally.

The results listed in Table 10, do not represent an exhaustive list of possible significant relationships. The analysis of covariance only shows those relationships to be significant when the variance associated with the mean value of a dependent variable at a specific level of an independent variable is uniquely different than the variance associated with the mean value of the same dependent variable at another level of the independent variable. Consequently, greater experimental precision could add to the list of significant relationships. The analysis of covariance also does not identify the mathematical relationship between an independent variable and a dependent variable as is done in regression analysis (Neter and Wasserman, 1974).

Table 10 shows that injector type is a significant contributor to resultant gas phase species mole fractions, temperature, and energy content (i.e. cold gas efficiency). The injector was found also to significantly effect carbon, nitrogen, and coal conversion to the gas phase. The conversion of elemental hydrogen in the coal to the gas phase was not found to be injector dependent. Oxygen/coal ratio and pressure were found to also significantly effect the particle and gas phase in the gasification process. Steam/coal ratio, however, was found only to significantly effect gas phase compositions.

The analysis of covariance suggests that conversion of hydrogen to the gas phase is not injector dependent. Graphical representations of hydrogen conversion relative to coal conversion; however, suggests that hydrogen conversion is injector dependent at coal conversion below 60% (Sowa, 1987). For most practical gasification applications coal conversion below 60% is not of interest. However, if char generation is desired, then this observation can be important.

Regression analysis was also performed to identify the mathematical relationship between the independent variables (O_2 /coal, pressure, steam/coal) and dependent variables (Sowa, 1987). The regression analyses were also used to construct simple second order models that could be optimized and compared to similar models developed from PCGC-2 modeling work. The regression analyses further reinforced the conclusions suggested by the analysis of covariance studies, as well as give additional insight.

Overall Coal Conversion. Figure 36 shows contour maps representing the coal conversion as a function of oxygen/coal ratio and steam/coal ratio for two different reactor pressures, 1.0 and 5.5 atmospheres for Injectors B, C and D. The extent of coal conversion was very different for each injector. The three injectors differed in their dependence on pressure and oxygen/coal ratio. Steam/coal ratio was not important for any of the three injectors as was expected from analysis of covariance results. Increasing oxygen/coal ratio increased coal conversion for every injector at both pressures. The effect of changing pressure on coal conversion was very injector dependent. The change in coal conversion with pressure appeared to correlate with the

TABLE 10

SUMMARY OF EXPERIMENTALLY SIGNIFICANT RELATIONSHIPS
DETERMINED USING ANALYSIS OF COVARIANCE

A. Definite Significant Relationships

<u>Independent Variable</u>	<u>Dependent Variables</u>
Injector	mole fractions: CO, CO ₂ , CH ₄ , H ₂ , H ₂ O conversion: C, N, coal cold gas efficiency exit gas temperature
O ₂ /coal	mole fractions: CO, H ₂ cold gas efficiency
Pressure	mole fractions: CO, CO ₂ , CH ₄ cold gas efficiency
Steam/coal	mole fractions: CO, CO ₂ , H ₂ , H ₂ O
Injector-pressure interaction	mole fraction: H ₂ conversions: C, coal

B. Probable Significant Relationships

<u>Independent Variables</u>	<u>Dependent Variables</u>
O ₂ /coal	mole fractions: CO ₂ , CH ₄ conversion: C, coal
injector-pressure interaction	mole fraction: H ₂ O cold gas efficiency

C. Possible Significant Relationships

<u>Independent Variable</u>	<u>Dependent Variable</u>
Pressure	mole fraction: H ₂ exit gas temperature
Injector-pressure interaction	mole fraction: H ₂ O conversion: N cold gas efficiency exit gas temperature

Figure 36. Quadratic regression model contour plots for overall coal conversion generated from experimental data as a function of O_2 /coal and steam/coal for two pressures 1.0 and 5.5 atm at a constant reactor fractional heat loss of 0.2 for injectors B, C and D.

degree of radial dispersion of the particle jet as it entered the gasifier. Injector B which neither fostered nor hindered primary-secondary mixing displayed no increase in coal conversion with increased pressure. Injector C which spread the particles throughout the reactor volume (forced primary-secondary mixing at the gasifier entrance) displayed increased carbon conversion with increased pressure. Injector D which compacted the primary particle jet into a tight column entering the gasifier, displayed poorer conversion with increased pressure. Injector B results might reflect what others have observed, that turbulent jet mixing does not become important until the injector Reynolds number is above 10000. Injector Reynolds numbers below 10000 are believed to still display diffusion controlled mixing (Perry, 1987).

A further explanation of the conversion results appears to be related to the trade-off between fuel-oxidizer stoichiometric ratios and the residence time of the particles in the intense flame region (i.e. flame length). The flame length did not change markedly with pressure for Injector C, only the residence time did. The flame length for Injectors B and D did change markedly with pressure. With Injector D, as the pressure was increased, the Reynolds number of the primary-secondary flow increased in the primary-secondary premixing chamber just above the combustion chamber. As the Reynolds number increased, the increased turbulent mixing of the two streams was offset by the increased density of the two streams in the premixing chamber. As can be seen in Table 10 (see Injector Characteristics), the primary jet density increased faster with pressure than the primary velocity decreased with pressure which caused the primary jet Reynolds number to increase. Consequently, the extent of premixing of the primary-secondary jet decreased with increasing pressure in Injector D. The better premixing of the secondary-primary jet for Injector D at low pressure, combined with a longer flame length, resulted in the highest coal conversion being displayed by Injector D at 1.0 atm pressure relative to itself at 5.5 atm pressure and relative to Injectors B and C at 1.0 atm pressure. At 1.0 atm pressure, Injector C, was penalized by its short flame length (particle residence time in the energy intense reaction zone) even though the particle distribution and primary-secondary mixing was superior to Injector D.

The coal conversion results indicate that the particle residence time in the intense reaction zone, the Reynolds number in the injector, the density of primary and secondary streams, the compactness of the primary coal jet and the degree of primary-secondary stream premixing were important in controlling the coal conversion process with Injectors B, C, and D. The compactness of the primary coal jet reflects directly on the magnitude of the local fuel-oxidizer stoichiometric ratio (or mixing) as the fuel passes through the intense reaction zone. The importance of either the local stoichiometric ratio or particle residence time in the reaction zone on coal conversion was very dependent on the injector. Consequently, optimum settings for one injector did not correspond to optimum settings for another. The highest measured coal conversions at the exit plane were measured using Injector C at 5.5 atm (ca. 80% on an ash included basis) and were at the same levels as coal conversions measured with a premixed flame, Injector A, at the same condition (Azuhata et al., 1986b).

Mapping Tests

Data Reliability. Three maps were created as part of the injector characterization study. Test conditions were shown in Table 8. Evaluating the reliability of mapping test data is more difficult than optimization exit plane data for three reasons. First, the assumption of complete mixing and a flat mass flux profile are not applicable in recirculating zones or where concentration gradients exist. The systematic errors that occur during sampling are hard to diagnose. Consequently, the correction of any measurements for air dilution becomes very difficult, if not impossible. The second problem was the ability to control the facility during operation. Only one axial plane was sampled in each firing. When a series of local position measurements from many different axial locations are combined to create a map, the variation in set point control from firing to firing adds to overall uncertainty. The third problem comes from the probe disturbing the flow by either modifying the local flow stream pattern or by sampling from too large of a local volume where strong concentration gradients exist. Further, not all radial positions were measureable due to probe plugging.

Measurement of molecular oxygen in the recirculation zones in amounts greater than 35 mole percent necessitated changes in the gas chromatograph temperature programs resulting in problems in the measurement of carbon dioxide. During all mapping tests, concentrations of carbon dioxide were approximated by subtracting all of the other measured gas mole fractions from one and attributing the remainder to carbon dioxide. The good repeatability in the measurement of the mole fractions of all gases except carbon dioxide from firing to firing justified this approach.

The correction of gas mole fractions for air dilution was not attempted for any mapping points measured during this study. During the atmospheric mapping tests of the swirled primary injector, Injector C, an error existed in the gas chromatograph program that controlled the measurement of molecular nitrogen. Only the measurement of molecular nitrogen was affected. In the reduction of the data from the Injector C atmospheric mapping tests (sample numbers 270-284), elemental nitrogen and sulfur were not used in any mass balances to estimate the local water mole fraction and progress variables, n , γ and f . The local molecular nitrogen concentration was estimated from progress variables found by forcing balances C, H, O, and Ar. Only the molecular nitrogen was adjusted and not molecular oxygen or argon concentrations. This adjustment of the molecular nitrogen was only possible because argon was being used as a window purge gas and not molecular nitrogen. No adjustments of measured gas concentrations were done on any of the other mapping measurements.

Table 11 presents the standard deviations of the set points throughout the mapping tests. The relatively large standard deviations for the oxygen/coal ratio results directly from the difficulty in accurately controlling the coal feed rate from firing to firing. The mapping data are useful in suggesting general trends in flame structure and species concentrations. However, problems in accurately determining the nature and extent of probe disturbances, controlling set points from firing to firing, and correcting gas measurements for any possible air dilution effects or other systematic errors during sampling should be considered when interpreting the mapping results.

TABLE 11

SUMMARY OF THE **STANDARD DEVIATIONS** IN THE EXPERIMENTAL SET POINT FOR
THE INJECTOR MAPPING TESTS WITH UTAH COAL

<u>Total Samples Collected</u>	<u>Coal Feed Rate (kg/hr)</u>	<u>Reactor Pressure (atm.)</u>	<u>O₂/Coal Ratio</u>	<u>Steam/Coal Ratio</u>
<u>(diffusion flame, parallel stream injection, Injector B)</u>				
23	2.47	0.1	0.07	0.0
<u>(diffusion flame, swirled primary, Injector C)</u>				
5	5.69	0.1	0.26	0.0
22	3.49	0.1	0.10	0.0
<u>(diffusion flame, impinging secondary, Injector D)</u>				
20	4.33	0.1	0.11	0.0

Local Coal Conversion. Figure 37 shows local coal conversion profiles for Injectors B, C, and D. Test pressure for the Injector C map was 1.0 atm. compared to 5.5 atm. for the other two injectors. This difference was necessary because the Injector C injector tip overheated at 5.5 atm after 20-30 minutes of steady operation.

Mapping tests show different flame structures for the three injectors. Even though Injector C was mapped at 1 atm pressure, the recirculation zone for Injector C was smaller than the recirculation zones for Injectors B and D at 5.5 atm. Only at the 22 cm axial position is the recirculation zone evident for Injector C. Injector B shows evidence of a strong recirculation zone persisting 52 cm from the injector tip. Injector D shows evidence of a strong recirculation zone persisting as far as 83 cm from the injector tip. The recirculation regions in Injectors B and D were characterized by high concentrations of oxygen (25-60 mole percent) and CO₂ (30-60 mole percent) and very low levels of CO (0-4 mole percent) and H₂ (0-1 mole percent). The recirculation region of Injector C had measureable amounts of oxygen (3-4 mole percent) but also significant amounts of CO (25-40 mole percent) and H₂ (3-13 mole percent) (see Appendix C). The high levels of oxygen measured in the recirculation regions of all three injectors explains why the coal conversion measured in these regions was very much higher than the coal conversion in the primary jet as well as the coal conversion measured at the reactor exhaust. Wall thermocouple measurements indicate that the regions of greatest heat release tended to be 30 ±10 cm from the injector tip for Injector C and 45 ±10 cm from the injector tip for Injectors B and D. These results suggest that the greatest amount of gas phase reactions with O₂ were occurring anywhere from 20-55 cm from the injector tip depending on the injector. Consequently, large concentrations of oxygen would be expected in the recirculation zone for all three injectors at those axial locations closer to the injector tip than the regions of intense heat release and reaction.

Figure 37. Overall coal conversion as a function of axial and radial position for injector B at 5.5 atm, injector C at 1.0 atm, and injector D at 5.5 atm from experimental mapping data. Basis: moisture free, ash included.

Nitrogen and Sulfur Pollutant Measurements

Measurements of the percents of the coal bound nitrogen and sulfur which were converted to gaseous species, and measurements of the nitrogen and sulfur gas phase species concentrations were made during the injector characterization testing. The objective was to more clearly understand the effect of injector configuration on the chemistry and formation of nitrogen and sulfur species during gasification. The key findings are discussed here and the discussion ties in with the discussion presented above on nitrogen and sulfur measurements. More detailed discussion is available in Nichols (1987). The nitrogen and sulfur measurements are tabulated in Appendix C.

Nitrogen Conversion. Nitrogen conversion measurements are shown in Figure 38 as a function of coal burnout (daf). Nitrogen conversion was not found to be dependent on pressure, or on steam/coal ratio. This compares to the previously reported gasifier data (Nichols, et al., 1987a) which show that increasing pressure from 1.0 to 10.4 atm had negligible effect on the nitrogen conversion. Nitrogen conversion is primarily dependent on the temperature in or near the flame zone where devolatilization occurs (since most of the fuel nitrogen is believed to be released during devolatilization). The temperature in this region is expected to be near the adiabatic flame temperature, and the adiabatic flame temperature is a weak function of pressure. Nitrogen conversion exceeded coal burnout for the levels of burnout measured in these tests. This also agrees with the previously reported gasification measurements (Nichols, et al., 1987). Nitrogen release from the coal has a higher degree of temperature dependency than overall mass release. Thus, at the high temperatures encountered in the pure oxygen blown gasifier flame, nitrogen release might be expected to exceed the release of carbon and/or total mass. Few gasifier data points were available at coal burnouts of less than 50%. It has been suggested (Pohl and Sarofim, 1976; Blair, et al., 1977) that nitrogen is bound in the coal primarily in aromatic rings, and that when devolatilization begins, about 10% of the coal mass is released before any nitrogen evolution occurs.

The level of nitrogen conversion was not found to vary significantly among the injector types, as coal burnout varied. This suggests a similarity of the kinetic processes for the evolution of nitrogen from the coal among the three injectors.

NO and TFN Formation. Measurement of nitric oxide (NO) and total fixed nitrogen (TFN) concentrations are plotted in Figures 39 and 40 for the three injector types. The term TFN is the sum of the species NH_3 , HCN, and NO. For the Diffusion Injector (B), effluent NO levels as high as 600 ppmv were measured at near atmospheric pressure. As pressure increased, the NO levels decreased dramatically. Concentrations of NO in gasification have been shown to be dependent on oxygen/coal ratio (Nichols, et al., 1987a; Price, et al. 1983). Some dependence of NO on oxygen/coal ratio was found here, but this effect was secondary in relation to the pressure effect. The effect of steam/coal ratio on NO levels was negligible. From results presented above, this observed influence of pressure is thought to be caused by the enhanced decay rate of NO which resulted directly from the increased pressure, and possibly to a lesser extent the increased residence time which resulted from maintaining the coal and oxygen feed rates relatively constant as pressure was increased. Space resolved NO measurements made at the mapping conditions for

Figure 38. Conversion of nitrogen and carbon to the gas phase during gasification of Utah bituminous coal ($O_2/\text{coal} = 0.40 - 1.25$, $H_2O/\text{coal} = 0.00 - 0.33$, pressure = 1.1 - 5.5 atm) straight line has a slope = 1.0. a) Injector B, b) Injector C, c) Injector D.

Figure 39. Effluent NO levels for various pressures, O_2 /coal ratios and H_2O /coal ratios; a) injector B b) injector C c) injector D.

Figure 40. Effluent Total Fixed Nitrogen (TFN) levels for various pressures, $O_2/coal$ ratios and $H_2O/coal$ ratios; a) Injector B, b) Injector C, c) Injector D.

TABLE 12

REPRESENTATIVE PCGC-2 INPUT PARAMETERS FOR THE FOUR INJECTORS

Parameter	Injector			
	A	B	C	D
Primary tube diameter (m)	0.006	0.005	0.003	0.005
Secondary tube diameter (m)	0.025	0.025	0.025	0.025
Chamber diameter (m)	0.203	0.203	0.203	0.203
Chamber length (m)	1.981	1.981	1.981	1.981
Primary gas (kg/s)	0.010	0.0025	0.0017	0.0025
Secondary gas (kg/s)	0.000	0.0078	0.0078	0.0078
Coal in primary (kg/s,dry)	0.011	0.0090	0.0090	0.0090
Primary swirl number	0.0	0.0	1.1	0.0
Primary turbulence intensity (%)	15.0	15.0	15.0	15.0
Primary temperature (K)	350.0	300.0	300.0	300.0
Primary mole fractions:				
Ar	0.059	0.828	0.756	0.828
H ₂ O	0.044	0.172	0.244	0.172
O ₂	0.897	0.0	0.0	0.0
Secondary swirl number	0.0	0.0	0.0	0.0
Secondary turbulence intensity (%)	0.0	15.0	15.0	15.0
Secondary temperature (K)	500.0	400.0	400.0	400.0
Secondary mole fractions:				
N ₂	1.000	1.000	1.000	1.000
Reactor pressure (kPa)	101.3	557.3	101.3	557.3
Side wall temperature (K)	950.0	1100.0	1100.0	1100.0
Particle solid density (kg/cu.m)	1350.0	1350.0	1350.0	1350.0
Heat of Formation, daf (kJ/kg)	-538.5	-538.5	-538.5	-538.5
Mass mean particle diameter* (μm)	0.0499	0.0476	0.0476	0.0476
Initial analysis:				
raw coal	0.914	0.914	0.914	0.914
ash	0.086	0.086	0.086	0.086
Elemental analysis (daf):				
C	0.805	0.805	0.805	0.805
H	0.060	0.060	0.060	0.060
O	0.115	0.115	0.115	0.115
N	0.016	0.016	0.016	0.016
S	0.005	0.005	0.005	0.005
Devolatilization parameters:				
A1 (1/sec x 10 ⁵)	3.7	3.7	3.7	3.7
E1 (J/kmol x 10 ⁸)	0.736	0.736	0.736	0.736
Y1	0.39	0.39	0.39	0.39
A2 (1/sec x 10 ¹³)	1.46	1.46	1.46	1.46
E2 (J/kmol x 10 ⁸)	2.51	2.51	2.51	2.51
Y2	0.80	0.80	0.80	0.80
Heterogeneous kinetic data:				
C-CO ₂ : A (m/sec K)	4894.0	1158.0	1158.0	1158.0
E (J/kmol x 10 ⁸)	2.60	2.59	2.59	2.59
C-H ₂ O: A (m/sec K)	1.33	1.33	1.33	1.33
E (J/kmol x 10 ⁸)	1.47	1.47	1.47	1.47
C-O ₂ : A (m/sec K)	0.478	1.03	1.03	1.03
E (J/kmol x 10 ⁸)	0.525	0.748	0.748	0.748

*continuous distribution simulated with 5 discrete sizes

Injector B showed that the centerline NO concentrations were 250 ppmv at 52 cm axial position, 2 ppmv at 83 cm, and 20 ppmv at 173 cm. Centerline NO measurements at the 22 cm axial location were not available. It is likely that the peak NO level in the gasifier occurred prior to the centerline measurement at 52 cm. No evidence was found that the peak NO level in the gasifier, using Injector B was less at 5 atm pressure than it was at atmospheric pressure.

Levels of TFN measured using Injector B are shown in Figure 40. Steam had no apparent effect on TFN levels. It appears that higher oxygen/coal ratios may have yielded lower TFN. This could be explained by the higher oxygen availability resulting in a greater fraction of the fuel nitrogen being converted to NO initially. This NO then would have been available to react with NH_3 (or an amine radical such as NH_2 or NH) to produce N_2 , thus reducing the TFN levels. Increasing the pressure tended to increase TFN levels. Since the only pathway for the removal of TFN species is by the previously mentioned reaction of NO with an amine species, these data suggest that at higher pressures, less NO was available for this to occur. In other words, these data suggest that at higher pressure, less NO is produced in and near the intense flame zone for the diffusion injector. Insufficient space resolved NO measurements exist to substantiate this suggestion. Furthermore, this would conflict with the previous discussion wherein it was noted that increasing pressure did not change the amount of NO produced in or near the flame.

Referring again to Figure 39, for the swirled primary injector (Injector C), effluent NO levels were not a function of pressure, oxygen/coal ratio or steam/coal ratio. Even at atmospheric pressure, effluent NO levels were in every case less than 25 ppmv, in contrast to the values of several hundred ppmv measured for the diffusion and the premixed injectors. This is likely due to more complete mixing caused by the dispersion of the primary stream containing the coal particles through the secondary oxygen stream. For the diffusion injector and the premixed injector, as well as for the impinging secondary injector to be discussed in the next paragraph, the primary stream was not dispersed or swirled. The momentum of the coal particles near the centerline could have caused pockets of high NO concentration and relatively low NH_3 and/or HCN concentration to remain near the centerline, thus resulting in high average exit NO levels. In the case of the swirled primary, such NO rich pockets would be less likely to exist because the particles are forced away from the centerline. Space resolved NO measurements for the swirled primary injector show a nearly flat profile of about 1000 ppmv NO at 22 cm axial location. This decays to about 600 ppmv NO by 52 cm, and less than 200 ppmv by 83 cm, and to less than 25 ppmv by the exit sampling location of 173 cm. It appears very likely that peak NO levels in excess of 1000 ppmv occurred prior to the 22 cm axial location.

Levels of TFN (Figure 40b) for the swirled primary injector ranged from 1500 to 8500 ppmv, not too different than the range of TFN levels for the ordinary diffusion injector. However, the data are widely scattered. The TFN levels showed no apparent correlation with pressure, oxygen/coal, or steam/coal. These TFN data were also compared to heat loss and coal feed rate, and no correlation was found.

Levels of effluent NO for the impinged secondary injector (Injector D) were also shown in Figure 39. At atmospheric pressure, effluent NO concentrations were as high as 400 ppmv, and decreased rapidly as pressure increased, similar to the behavior observed for the ordinary diffusion injector. Again, this implies that impinging the secondary gas stream into the primary particle stream does not have the same effect as directing (or swirling) the primary particle stream into the secondary gas stream. The TFN levels in Figure 40c for the impinged secondary injector range from 2,000 to 10,000 ppmv. TFN levels appear to show a minimum with increasing pressure, at near 3 atm. In particular, TFN levels were highest at the highest pressure level. As discussed for the ordinary diffusion injector, this may suggest that at higher pressure, less NO is produced in or near the flame, thus providing less opportunity for the conversion of TFN to N_2 . Higher oxygen/coal levels resulted in lower TFN levels in most cases. This is again explained by higher oxygen yielding higher NO levels, thus providing more opportunity for the reaction of NO with an amine species (or radical) to N_2 . Steam/coal ratio apparently had no effect on NO or TFN levels for this injector.

The following conclusions were reached concerning nitrogen release and nitrogen species formation during the injector characterization gasifier tests. 1) Nitrogen conversion exceeded coal burnout (daf) as has been consistently observed in other gasification tests, and did not depend on injector type (considering Injectors B, C, and D). 2) The swirled primary injector (Injector C) produced the lowest levels of NO in the gasifier effluent, and these levels were independent of the test variables. This was thought to be due to the high degree of mixing that occurred. 3) The levels of TFN ($NO + NH_3 + HCN$) were not greatly different among injectors. Levels of TFN ranged from approximately 2,000 to 10,000 ppmv. 4) TFN levels appeared to decrease with increasing oxygen level. This was consistent with the fact that the only pathway for removal of TFN to N_2 is via reaction of NO with HCN or NH_3 . 5) Adding steam to the gasification process had no significant impact on the nitrogen species formation for any of the three injectors.

Sulfur Pollutant Measurements

The bulk of the gas phase sulfur was found as H_2S , with lesser amounts of COS, CS_2 and SO_2 measured. Nearly all of this H_2S was found in the gas portion of the gas-liquid-solid water quenched sample. On the order of 10% of the H_2S was found dissolved in the probe quench water as $S^{=}$ ion. These findings are consistent with the sulfur measurements made during other gasification tests and discussed above. Levels of H_2S were not noted to be significantly affected by injector type.

PCGC-2 Modeling for Injector Characterization Study

Optimization Tests. The four different injectors illustrated in Figure 34 were modelled with the PCGC-2 code, prior to testing. Oxygen/coal ratio, steam/coal ratio and reactor chamber pressure were varied according to a Box-Behnken statistical design (Hurst et al., 1986; and, Smith et al., 1986). Table 12 lists representative PCGC-2 input parameters for the four injectors, with a comprehensive list found in Sowa (1987). Table 13 summarizes the modeling computations completed. All cases were run using a heat loss factor of 0.2.

TABLE 13

SUMMARY OF PCGC-2 MODELING TEST CONDITIONS, AND NUMBER OF CONVERGED CASES

<u>Test Series</u>	<u>Total Cases Converged</u>	<u>Coal Feed Rate (kg/hr)</u>	<u>Reactor Pressure (atm.)</u>	<u>O₂/Coal Ratio</u>	<u>Steam/Coal Ratio</u>
<u>Utah coal (premixed flame, parallel injection, Injector A)</u>					
optimization	13	40	1-10	0.7-1.15	0.0-0.3
<u>Utah coal (diffusion flame, parallel injection, Injector B)</u>					
optimization	13	33	1-10	0.7-1.0	0.0-0.3
comparison to experimental map	1	33	5.5	0.85	0.0
<u>Utah coal (diffusion flame, swirled primary, Injector C)</u>					
optimization	13	33	1-10	0.7-1.0	0.0-0.3
comparison to experimental map	1	33	1.0	0.85	0.0
<u>Utah coal (diffusion flame, impinging secondary, Injector D)</u>					
optimization	17	33	3.25-10	0.7-1.0	0.0-0.3
comparison to experimental map	1	33	5.5	0.85	0.0

The oxygen/coal ratio range studied with Injector A was larger than the range used with the other three injectors. Injector A predictions were done using two different statistical models, a split level design and a Box-Behnken design. The split level design used two levels of reactor pressure and steam/coal ratio and four levels of O₂/coal ratio. The Box Behnken design used three levels of O₂/coal, steam/coal and reactor pressure. The results from the two different test designs were correlated using statistical regression models and evaluated on OPTDES.BYU, a nonlinear optimization method (Parkinson, et al., 1984). The Box Behnken test design was found to be superior to the split level design because of the orthogonality of the points sampled in design space. The orthogonality of the Box-Behnken design allowed for quadratic interpolating functions to be created that could be used to explore design space without having the regression equation strongly biased by the O₂/coal ratio at the expense of reactor pressure and steam/coal ratio. More details of this work can be found in Hurst, et al. (1986) and Sowa (1987).

The range of reactor pressures examined for Injector D was smaller than the pressure ranges used with the other three injectors. As the reactor pressure decreased in magnitude for Injector D, obtaining code convergence became increasingly difficult. No atmospheric case was converged for Injector D. The cause of the numerical instabilities for the Injector D atmospheric cases has not been conclusively determined. The atmospheric iso-contour plots which follow for Injector D are extrapolations from the PCGC-2 results using statistical regression models.

General Trends. Analysis of variance was used to determine which dependent and independent variables had significant relationships predicted by PCGC-2. The same variables were investigated using experimental optimization results. Table 14 shows significant relationships. Since PCGC-2 predictions are not stochastic, determination of significant effects was much easier than the experimental determination of significant effects. Consequently, no entries for probable and possible significance are shown in Table 14 as was done in Table 10.

Unlike the general trends from the experimental results, significant difference between injectors was only displayed in the gas phase mole fractions of CO_2 , H_2 and H_2O , and the exit gas temperature. All PCGC-2 particle phase conversions showed no dependence on injector type. Oxygen/coal ratio and pressure, however, demonstrated a significant effect on almost all gas phase and particle phase properties considered. The significant effect of pressure on the predicted water mole fractions and solids conversion is contrary to the experimental results. PCGC-2 predictions which demonstrated significant interaction with steam agree very well with the experimental results.

Coal Conversion. Figure 41 shows contour maps of coal conversion as a function of O_2 /coal ratio and steam/coal ratio for two different reactor pressures, 1.0 and 5.5 atmospheres. The coal conversions are on an ash included basis. Coal conversions of 91% correspond to 100% conversion of the organic material.

Like the experimental results, coal conversion had either no dependence on steam/coal ratio (Injectors B and C) or very slight dependence on steam/coal ratio (Injector D). Like the experimental results, Injector D showed the highest conversions at 1.0 atm pressure and Injector C at 5.5 atm. All three injectors had operating conditions within the specified variable ranges where PCGC-2 predicted complete conversion of the coal organic matter. The PCGC-2 predicted regions of optimum conversion for Injectors B, C and D agreed well with the experimental results namely at the maximum oxygen/coal ratio. Unlike the experimental results, the coal conversion values for all three injectors were all very similar in magnitude, and the effect of pressure on coal conversion did not agree with the experimental measurements. Finally, and probably most significant, the magnitude of conversion was much greater in all PCGC-2 predictions than was measured experimentally. In some cases, PCGC-2 predicted coal conversions more than two times greater than were observed experimentally (compared Injector D results at 5.5 atm pressure, Figure 41). The PCGC-2 predictions suggested that the overall flame structure of the three Injectors B, C and D was not radically different between injectors. The experimental results, however, suggested just the opposite.

Because PCGC-2 assumed that all elements in the coal were converted to the gas phase at the same rate, the coal carbon conversion and coal hydrogen conversion were predicted to occur the same as the coal. The unique hydrogen conversion behavior compared to carbon conversion observed experimentally was not predictable using PCGC-2.

The discrepancy between PCGC-2 predictions and experimental measurements may be attributed to several factors related to mixing. First, the Reynold's numbers from the experimental work ranged from 1500-3000 when predicted using

TABLE 14

SUMMARY OF SIGNIFICANT RELATIONSHIPS DETERMINED USING
ANALYSIS OF VARIANCE ON PCGC-2 PREDICTIONS

Definite Significant Relationships

<u>Independent Variable</u>	<u>Dependent Variable</u>
injector	mole fractions: CO_2 , H_2 , H_2O exit gas temperature
O_2/coal	mole fractions: CO , CO_2 , CH_4 , H_2 , H_2O conversion: C , H , N , coal cold gas efficiency exit gas temperature
Pressure	mole fractions: CO_2 , CH_4 , H_2 , H_2O conversion: C , H , N , coal coal gas efficiency exit gas temperature
Steam/coal	mole fractions: CO , CO_2 , H_2 , H_2O exit gas temperature

Figure 41. Quadratic regression model contour plots for overall coal conversion generated from PCGC-2 results as a function of O₂/coal and steam/coal for two pressures 1.0 and 5.5 atm at a constant reactor fractional heat loss of 0.2 for injectors B, C and D.

uncorrected thermocouple temperature measurements at the gasifier exit and based upon the exhaust gas mass flow rate and reaction chamber inside diameter. These Reynold's numbers indicate that the experimental flows were most likely in the transition region and likely did not have the same mixing intensity that a fully developed turbulent flow would have. PCGC-2 assumes that the flow is fully turbulent. Second, cold flow work performed by Lindsay (1986) as well as work by Rasband (1987) comparing PCGC-2 predictions to experimental work has suggested that the k- ϵ turbulence model used in PCGC-2 predicts the overall mixing to occur somewhat more rapidly than measured. Further, no attempt was made to further increase the number of radial nodes in the primary and secondary region or to determine the effect of node spacing on the predictions.

In addition, the differences in magnitude between predicted and measured coal conversion values may be related to at least four factors: 1) the heat loss factor used in PCGC-2, 2) the devolatilization parameters used in PCGC-2, 3) the rate of mixing, and 4) the heterogeneous char reaction rates. Brown (1985) used a heat loss factor 0.5 to obtain good agreement between the experimental measurements and PCGC-2 for atmospheric gasification using Injector A. In modeling Injectors B, C, and D, using a higher heat loss factor would lessen the extent of predicted conversion, however, a higher heat loss factor was not justified by the experimental data since the measured overall heat loss averaged 0.18 for all of the experimental optimization tests which corresponds to a heat loss factor of 0.15-0.35. The average value of the experimental heat loss would have been decreased if the bare thermocouple measuring the exhaust gas temperature were corrected for radiation and conduction losses. A higher exit gas temperature would have increased the gas sensible heat term and reduced the estimated heat loss. Injectors B, C and D were modeled using a heat loss factor of 0.2.

The devolatilization parameters were taken directly from Ubhayaker et al. (1976). No attempt was made to modify either the devolatilization reaction rate parameters or the extent of reaction parameters. The bulk of the coal conversion (60-70% of total coal mass) was directly attributed to coal devolatilization.

Predicted fast mixing could cause greater predicted than measured coal conversion by prematurely mixing oxidizer and fuel where the reaction temperatures were the hottest instead of spreading out the flame and the fuel heat release. More will be discussed on this issue when the PCGC-2 predictions are compared to the experimental maps. No heterogeneous reaction rate parameters were available for the specific coal modeled, in this case a Utah bituminous coal. The Utah coal used during this study would have been best modeled as a high-volatile B bituminous. Even when parameter data are available, parameters must be used in temperature regimes far removed from temperature regimes where the experimental rate data were measured that estimated the parameters in the first place. Baxter (1986) has shown that the predicted reaction rate at very high temperatures can vary by more than an order of magnitude depending on the regression method used to estimate the kinetic parameters.

Comparison to Mapping Tests. Table 14 showed the model parameters used for the mapping predictions. Figure 42 shows predicted temperature profiles for the three injectors. The peak predicted temperature is located between

Radial Position From Centerline (cm)

Figure 42. Overall temperature (degrees kelvin) as a function of axial and radial position for Injector B at 5.5 atm, Injector C at 1.0 atm, and Injector D at 5.5 atm from PCGC-2 predictions.

4.5 to 28.0 cm from the injector tip for Injectors B and D, at 5.5 atm pressure and 10-55 cm for Injector C at 1 atm. Experimentally, the region of greatest heat release (which most likely correlates with position of maximum flame temperature) was measured by wall thermocouples to occur at 45 cm $\pm$ 10 cm from the injector tip at 5.5 atm and 20-40 cm at atm pressure. These comparisons indicate that predicted intense heat producing reactions for Injectors B and D occur too close to the injector tip. The temperature predictions of Injector C seem to correspond well with experimental observations.

Figure 43 shows profiles for coal conversion for all three injectors. For Injectors B and D, the regions of greatest particle mass flux occur outside of the recirculation zone and concentrated towards the reactor centerline. Experimentally, the recirculation zones of injectors B and D consisted entirely of CO₂ and O₂ with very little or no CO measured (see Appendix C). The high oxygen concentrations in the recirculation zones created a region of high coal conversions exceeding exit plane values like is shown in the Injector C predictions. Also no regions of high coal conversion on or near the reactor centerline around 20 cm from the injector tip were measured experimentally. The Injector C coal conversion map more closely parallels what was observed in Injector B. Experimentally, Injector C showed much flatter profiles at the 52 cm position than was predicted. However, of all of the injector predictions Injector C comes closest in agreement to measured values.

Subtask 1.3 - Cold Flow Jet Mixing Tests

Introduction

Cold flows resembling those found in the laboratory gasifier were studied to gain information about the basic flow processes of gasification without the complications of chemical reaction. Laser Doppler velocimetry (LDV), a nonintrusive flow diagnostic technique, was used to make in-situ measurements of mean velocity components and turbulence intensities in the isothermal confined-jet flows. The LDV data were used to evaluate and refine the fluid mechanics portions of the PCGC-2 code and to develop an understanding of swirl phenomena and other effects. The LDV measurements were also used to provide inlet turbulence and velocity data as initial conditions for PCGC-2 cases.

Like the gasifier of this study, many combustion-related systems employ confined, coaxial jets. Several researchers have investigated these flows (e.g., Ribeiro and Whitelaw, 1980; Champagne and Wagnaski, 1970; Habib and Whitelaw, 1979; Owen, 1976; Smoot, 1976; Dixon, et al., 1983). While flows specifically applicable to pulverized-coal reactors have received less attention, valuable insight can be gained from the general body of research with coaxial jet systems. The phenomena associated with swirl in such flows has also received much attention in recent years. Lilley (1977), Gupta et al. (1984), and Sloan (1985) provide excellent reviews on swirl in practical flow systems. Specific studies of note include those of Ribeiro and Whitelaw (1980), Claypole and Syred (1982), Roback and Johnson (1983), Altgeld et al. (1983), and Chigier and Dvorak (1974). Work directly related to coal combustion flows includes that of Webb and Hedman (1982) and Jones et al. (1984), who made LDV measurements of axial velocity in a cold, simulated

Figure 43. Overall coal conversion as a function of axial and radial position for injector B at 5.5 atm, injector C at 1.0 atm, and injector D at 5.5 atm from PCGC-2 predictions. Basis: moisture free, ash included.

pulverized-coal combustor flow. Intrusive probes were also used to study particle and gas mixing in several earlier studies of simulated pulverized-coal flows (Memmott and Smoot, 1978; Tice and Smoot, 1978). The present study of simulated gasifier flows is part of a broad experimental effort which will lead to direct LDV and CARS measurements in reacting pulverized-coal gasifiers.

The application of experimental data to computer models is crucial to the development and refinement of such models. In spite of the large amount of data available in the literature, model development has far outstripped the available data for comparison (Smoot and Hill, 1983; Reynolds and Cebeci, 1978). Much of the data from the past has been collected with intrusive probes which in some cases may seriously distort the flow being measured (Gouldin, et al., 1983). Furthermore, most studies have not included measurements at the inlet. Documentation of the inlet boundary condition is often needed if experimental data are to be properly applied to model development (Abujelala and Lilley, 1983; Sturgess, et al., 1983).

Test Facility

LDV System. A single-frequency backscatter-mode LDV system (TSI Model 9100-6) with a 120 mW argon-ion laser was used in this study. All measurements were made with frequency shifting from a Bragg cell. Signals were processed with a counter (TSI model 1990A) and data sets from each measurement were stored on and reduced by an HP1000 computer. A 'homemade' interface and signal driver system was used to multiplex and transmit the digital data to the computer across a 300 foot distance. Details are given in (Webb and Hedman, 1982; Jones, et al., 1984; Lindsay, et al., 1986).

Following the completion of the simulated gasifier measurements with the single-frequency LDV, the LDV system was disassembled and a new two-frequency system was installed. The two-frequency system employs the same laser and many of the same optical components. Details of the system and the data acquisition and reduction software are given by Lindsay (1986). The two-frequency system offers many advantages over the previous LDV, including simultaneous measurement of two orthogonal velocity components, determination of Reynolds stresses, powerful bias correction and elimination strategies, and accurate measurement of time-between-data values to permit proper spectral analysis.

The two-frequency system and the newly written software for it were tested by generating optical Doppler signals of known frequency using a frequency shifter and a stationary light-scattering surface. The data were successfully transmitted by the LDV system across the entire data path consisting of a signal processor, a master interface, 125 feet of cable, a signal driver, and a high-speed DMA board in a MicroVAX II computer. The binary data were then converted to decimal form and reduced. The measured frequency values were within roughly 0.2% of the known input frequency for all frequencies used (10kHz to 5MHz). The accuracy of the system was thus successfully demonstrated.

Flow Chamber. The horizontal flow chamber used in this study simulates the cylindrical coal gasifier used for studies of reacting flow at this laboratory (Soelberg, et al., 1985). Figure 44 depicts the flow facility and

Figure 44. Schematic of the cold-flow facility and LDA system.

the LDV system. Figure 45 shows the inlet configuration of the flow facility. The flow inlet consists of an annular tube for the secondary stream (with annular diameters of 1.6 and 2.7 cm) around a central tube for the primary stream (i.d. 1.0 cm). The primary jet flows from a pipe with a blunt lip, 3 mm thick which simulates the ceramic primary stream tube that was used in the reacting gasifier system of Soelberg et al., (1985). A 35-degree half-angle diverging nozzle 4 cm in length leads the streams into the 20-cm diameter mixing chamber. The chamber is 0.9 m long and terminates with a conical contraction to a 13 cm diameter pipe (length 35 feet) through which the flow exits into the atmosphere. Swirl in the secondary stream was generated by a modified movable-block device (Beer and Chigier, 1972). Details of the swirl block are shown by Lindsay (1986). The air was seeded with micron-sized alumina or titanium dioxide particles. Seed particles were introduced independently into both streams. Fluidized beds seeded the flow in most cases.

Test Program and Procedures

Test Matrix. LDV measurements were made in a variety of flow cases in order to observe the effects of different inlet conditions. A gasifier cold-flow case can be specified by three inlet parameters: 1) the mean primary stream inlet velocity (V_p), 2) the mean secondary stream inlet velocity (V_s), and 3) secondary swirl number (S). For the cases of most interest, primary and secondary inlet velocities were chosen so that inlet Reynolds numbers corresponded to those of Soelberg, et al. (1985) for a reactive, entrained-flow, pulverized-coal gasifier. In these cold flow cases, V_p was set at 34 m/s, giving a primary stream Reynolds number of 19,000, and V_s was set at 5 m/s, giving a secondary stream Reynolds number of 3000. The corresponding air mass flow rates at 20 C and 0.85 atm are, respectively, 2.8 and 1.9 g/s. A factorial design for the test program was established in which V_p had three levels (17, 34, and 51 m/s), V_s had three levels (0, 5, and 8 m/s), and S had three levels (0, 0.5, and 0.9). The test program required that axial and tangential velocity profiles be obtained at several axial stations for each flow case. Replicate measurements were also conducted to check experimental error and to permit the statistical analysis of results between flow cases.

In this report, a given flow case is designated with the notation $\langle a, b, c \rangle$ where a and b are the primary and secondary stream velocities, respectively, in m/s, and c is the secondary swirl number. For instance, the non-swirling case most similar to the Soelberg gasification case is designated as case $\langle 34, 5, 0 \rangle$.

With the above choices for inlet conditions, the amount of swirled flow from the secondary stream was not enough to induce central recirculation zones (some strongly swirled flow cases were created by using swirled secondary flow only, but these were not of direct interest in this study). The swirled flows therefore fall under the category of weakly swirling flows (Gupta, et al., 1984). Under normal operating conditions, strong swirl is not possible in the laboratory gasifier.

Experimental Methods. Before starting the test program, work was done to ensure that acceptable measurement techniques would be used in the flows of interest. Theoretical considerations were combined with a series of LDV tests to establish criteria for settings of frequency shift, electronic filters,

Figure 45. Schematic of the inlet assembly in the cold flow facility.

gain, and other electronic settings as a function of the local flow properties. Based on this preliminary work, frequency shifts of 2-5 MHz were used for axial velocity measurements in recirculation zones and for many of the tangential velocity measurements. Lower frequency shifts (0.1 to 1.0 MHz) were generally used for axial velocity measurements in jet cores. In most cases, the TSI counter was used in the 16 cycle mode, although 32 cycles were sometimes required to obtain acceptable signal quality at frequency shifts of 5 or 10 MHz. Further processor setting details are given in Lindsay (1986).

Bias effects were also of concern for the data rates and sampling procedures used in this study (Buchhave and George, 1979; Durao, et al., 1980; Adams, et al., 1986; Stevenson, et al., 1982). Standard procedures to reduce bias effects included periodic sampling or random sampling with time-weighting of the mean and rms velocities (Adams, et al., 1986; Stevenson, et al., 1982; Durst, et al., 1981). Time-weighting was frequently based on particle residence times or time-between-data values. Due to limitations of the 'homemade' interface system, the LDV system could not be operated in total burst mode, which precluded the measurement of particle residence time in the probe volume (Adams, et al., 1986). Time-between-data values also could not be measured. Periodic sampling was not used and would have been impractical because of the generally low data rates encountered in this study.

An approximate time-weighted averaging method was employed in which the weighting factor, t_i , is given by

$$t_i = N / \{ |f_s| + |f_d| \}, \quad (6)$$

where N is the number of Doppler cycles, f_s is the frequency shift and f_d is the pure Doppler shift due to the velocity of the moving particle. In total burst mode, this method would give results that would be independent of the frequency shift (Buchhave and George, 1979; Adams, et al., 1986). In single burst mode, however, this weighting procedure is dependent on frequency shift. This was partially remedied through the use of criteria for frequency shifting and for the averaging procedure (number-weighting versus approximate time-weighting) as a function of the flow regime being measured. Low frequency shifts (0.01-1 MHz) were used for axial velocity measurements in the jet core regions, higher shifts (1-5 MHz) were used for axial velocity measurements in shear regions and recirculation zones, and high shifts (often 5-10 MHz) were used for tangential velocity measurements. Based on preliminary flow measurements and on a computational analysis of bias effects, approximate time-weighted averaging was chosen for axial velocity measurements in the core of the flow, where axial velocities were positive and dominant, and number-weighted averaging was generally used for tangential velocity measurements and for axial velocity measurements in the weak recirculation zones. A more complete discussion of the data reduction methods and their usefulness and accuracy is given in Lindsay (1986).

Results and Discussion

Simulated Gasifier Profile Measurements. Measurements in 20 flow cases were made, 15 of which correspond to cases from the 3x3x3 factorial design.

TABLE 15

AXIAL LOCATION OF PROFILE MEASUREMENTS FOR SIMULATED GASIFIER FLOW CASES
 ("I" designates measurements at the inlet plane. The notation <a,b,c> for flow cases means that
 "a" is the primary inlet velocity in m/s, "b" is the secondary inlet velocity, and "c" is the secondary
 swirl number)

<u>Set</u>	<u>Case</u>	<u>Primary Reynolds No.</u>	<u>Secondary Reynolds No.</u>	<u>Axial locations (cm) for:</u>	
				<u>Axial Vel.</u>	<u>Tangential Vel.</u>
1.	<34,5,0>	19,000	3,000	1, 11, 20, 27, 43, 57	1, 11, 20, 27, 43
2.	<34,5,0.5>	19,000	3,000	1, 11, 20, 27, 43	1, 11, 20, 27
3.	<34,5,0.9>	19,000	3,000	1, 11, 20, 27, 43, 57	1, 11, 20, 27, 43
4.	<34,0,0>	19,000	0	1, 11, 20, 27, 43	1, 20, 43
5.	<51,7,0>	28,500	4,200	1, 11, 20, 57	1, 11, 20
6.	<51,7,0.5>	28,500	4,200	1, 20, 27	1, 11, 20
7.	<51,7,0.9>	28,500	4,200	1, 20, 57	1, 11, 20, 43
8.	<51,0,0>	28,500	0	1, 11, 20, 43	1, 11, 20, 43
9.	<17,5,0>	9,500	3,000	1, 11, 20	11, 20
10.	<17,5,0.5>	9,500	3,000	11, 20	11, 20, 27
11.	<17,5,0.9>	9,500	3,000	20	11, 20
12.	<34,7,0.9>	19,000	3,000	11, 20	20
13.	<34,7,0.5>	19,000	4,200		20
14.	<51,5,0.5>	28,500	3,000		27
15.	<51,5,0.9>	28,500	3,000		27
16.	<0,5,0.5>	0	3,000		11
17.	<0,5,0.9>	0	3,000		20, 27
18.	<0,7,0.9>	0	3,000	20	20
19.	<51,0,0>	28,500	0	11	
20.	<60,0,0>	34,000	0	11	

Table 15 lists the flow cases studied and the axial locations at which axial and tangential velocity measurements were made. Over 100 sets of useful velocity profile measurements were made, each with an average of 40 measurements at various radial locations. Profile measurements were made across most of the diameter of the flow chamber, in order to check flow symmetry. Replicate profile measurements (done on different days) were made to estimate the variance due to outside effects such as changes in atmospheric pressure, variance in flow rate and swirl settings, and errors in manually repositioning the LDV axis at a given axial location. The reproducibility of velocity profiles was acceptable. For instance, replicate centerline mean axial velocity values were, on the average, reproducible within 6%. Within each profile measurement series, replicate measurements at given points were also made to check experimental error and flow stability. In some cases, the variance of replicate measurements was on the order of 1-3 times the minimum expected variance due solely to finite sample sizes. However, much larger variance was sometimes observed, as described below.

Flow Unsteadiness. While turbulent flows are truly transient, the flow properties averaged over a sufficient time can be highly reproducible. Many turbulent flows show this property which will be defined as "steadiness" in this report. Since the turbulent time scale is often on the order of milliseconds, an averaging time on the order of a few seconds is usually sufficient to observe steadiness. Since the LDV measurements typically were averaged over 20 to 60 seconds, steadiness was expected in the data. However, significant long-term unsteadiness was encountered in some cases. This behavior made the interpretation of the data more difficult.

Unsteady flow regimes were often encountered beyond the 20 axial locations for flows with swirl. In such cases, successive LDV measurements at a single point showed fluctuations on the order of 10-100% in mean velocity values. Fluctuations in the corresponding rms velocities rarely exceeded 15%, however. In regions of unsteadiness, multiple measurements were required to estimate true mean properties. No simple periodicity was observed in the replicate LDV measurements. Unsteadiness was observed for flow cases with primary flow only and with primary and secondary flow together. The nature of the unsteadiness was reproducible - i.e., the degree of scatter and the relation between replicate mean and rms velocities could be reproduced.

This unsteadiness was associated with the low Reynolds numbers, ranging from roughly 500 to 2,500 in the mixing chamber for the flow cases of this study. While turbulence was indicated in all measurements, flow transitions associated with relaminarization (oscillations between metastable states) apparently occurred in some parts of some flow cases. Figure 46 shows portions of velocity time series taken from LDV measurements. Consecutive LDV measurements were begun about every 90 seconds, with each measurement lasting from 30-60 seconds. Evidence of sudden flow transitions can be seen.

Flow unsteadiness most affected the tangential velocity measurements. Even when the unsteadiness in the axial direction appeared minor, the weak tangential velocities could show significant fluctuations. These fluctuations were on the order of 0.1 m/s, which was usually only 10% or less of the local rms velocity. However, such fluctuations were troublesome because the mean tangential velocities past the 11 cm location rarely exceeded 0.5 m/s.

Figure 46. Two examples of sequential LDA tangential velocity measurements in unsteady flow regimes. Each data point is a 60-second average. An interval of roughly 30 seconds lies between each measurement.

Unsteadiness was most severe in the swirled flow cases which became mixed more rapidly than the unswirled flows. A strong central jet in a poorly mixed flow apparently stabilizes the flow, but as the axial velocity profile becomes flatter, transitions can occur. However, in strongly swirled flows with central recirculation zones, flow unsteadiness was not apparent, even when the chamber Reynolds number was as low as 500. The central recirculation zone may have stabilized the turbulent flow in this case.

The finding of unsteady flows in the cold-flows of the simulated gasifier may have ramifications for reacting gasifier flows. The chamber Reynolds numbers of the flows of previous and current laboratory gasification studies are estimated to be in the 1500-4000 range. With such Reynolds numbers, unsteady transition effects are possible. Occasional series of replicate measurements are recommended to examine the steadiness of local gasifier properties.

Test Results. Flow symmetry about the centerline was sufficient to represent the results with radial profiles only. Profiles for case <34,5,0.9> are thus shown in Figures 47-50. Over thirty similar profile sets for other flow cases are given by Lindsay (1986). Both mean and rms velocity profiles for tangential and axial components are shown. The plots were generally drawn point-to-point, with a French-curve approach employed to maintain smooth lines. Vertical bars on the profiles show the range of replicate measurements at selected radial locations. Small numbers at the sides of the bars indicate how many replicate measurements are included in each range. The range bars, which are roughly equivalent to 95% confidence bands, show the combined effect of experimental error, uncertainty due to flow unsteadiness, and variance in profile replications from different runs. The data in each range include measurements on both sides of the flow centerline, so any errors due to asymmetry are also included.

The axial velocity profiles in Figure 47 show that the coaxial jets merge into a single central jet which spreads and approaches the fully developed state at the 57 cm location. Recirculating flow is present at all locations except possibly the last (measurements could not be made within 1 cm of the wall because of optical noise). The magnitude of the maximum negative velocity changes only weakly with axial location. Significant unsteadiness in the flow was encountered at the 27 cm axial location, as is reflected in the large range bars. The corresponding tangential velocity profiles in Figure 48 show a fairly rapid decay in tangential velocity as the axial velocity profiles flatten. The maximum tangential velocity of 3.5 m/s at the inlet has decreased to a maximum of 0.2 m/s after 27 cm. Each profile is closely linked, of course, to the corresponding axial velocity profile. At the 43 cm location, for instance, where the axial flow is spread out into a mostly flat profile, the tangential velocity profile has a forced vortex shape across most of the duct. The maximum tangential velocity is also 0.2 m/s.

Flow unsteadiness made determination of the tangential velocity profiles difficult. Unsteadiness was severe at the 11-27 cm axial locations, and is reflected in the large range bands for those profiles. At the 27 cm axial location, such large fluctuations in tangential velocity were observed beyond about the 3.5 cm radial location that the profiles shape in that region is unknown. The profile shape within 4 cm of the wall at the 20 cm axial location is also uncertain, though it appears that the mean tangential

Figure 47. Axial velocity profiles for case <34,5,0.9>. Vertical bars show the range of the data at selected radial locations, including results from replicate profile measurements and results from both sides of the axis of symmetry. Numbers at the sides of the bars indicate the number of data points included in the range.

Figure 48. Tangential velocity profiles for case $\langle 34, 5, 0.9 \rangle$. Vertical bars show the range of the data taken at selected radial locations, including results from replicate profile measurements and results from both sides of the axis of symmetry. Numbers at the sides of the bars indicate the number of data points included in the range. The dashed section of the profile at 27 cm is the assumed profile shape in a region where the unsteadiness was too severe to determine the real profile shape.

Figure 49. Axial rms velocity profiles for case <34,5,0.9>. Vertical bars show the range of the data at selected radial locations, including results from replicate profile measurements and results from both sides of the axis of symmetry. Numbers at the sides of the bars indicate the number of data points included in the range.

Figure 50. Tangential rms velocity profiles for case <34,5,0.9>. Vertical bars show the range of the data at selected radial locations, including results from replicate profile measurements and results from both sides of the axis of symmetry. Numbers at the sides of the bars indicate the number of data points included in the range.

velocity there may be near zero. Unsteadiness at the 43 cm axial location was also encountered, but was much less severe.

Examination of axial and tangential rms velocities in Figures 49 and 50 shows the axial rms velocities are consistently higher (an exception occurs at one radial location in the secondary inlet stream near the primary wall). Both rms velocity components at the centerline increase rapidly from the low values at the inlet to values roughly three times as great at the 11 cm axial location. The profiles decay to fairly uniform values towards the end of the chamber. In the primary inlet stream, which is fully developed, the maximum rms velocities occur near the wall. Once turbulent mixing occurs, the maximum rms velocity is at or near the centerline, with a minimum in the outer recirculation zone. A local maximum probably occurs near the chamber wall, but measurements could not be made close enough to the wall to observe these effects.

From a statistical analysis (Lindsay, 1986) effects of key variables on flow properties were evaluated. The most important variable was the swirl level, followed by the $V_p \times S$ interaction. Even weak swirl therefore significantly affects the axial velocity decay (and hence the mixing rates) for the flow cases studied. Effects of V_p and V_s were also significant.

Inlet Measurements. Knowledge of the initial boundary conditions is often important if data are to be applied to a predictive code. In some cases, the use of assumed or theoretical inlet conditions can lead to serious errors in the predictions (Gouldin, et al., 1983; Abujelala and Lilley, 1983; Hendricks and Brighton, 1975; Capp, and George, 1982). LDV measurements at the inlet plane were therefore included in this study.

A recessed optical access port was added in the inlet assembly after the downstream profile measurements had been completed (see Figure 45). In this way, the possible inlet perturbation due to the presence of the port would not affect the downstream measurements. The pipe for the primary stream was moved upstream so that the laser beams would just miss the end of the pipe. This also permitted inlet profile measurements to be made across both streams without additional equipment modifications. These profiles were only made across a radial section because scattered light from the remote secondary stream wall interfered with measurements made beyond the inlet centerline. It is recognized that the portion of the inlet flow in which these measurements were made may not correspond exactly to the flow at the beginning of the expanding nozzle, but no significant difference was expected. For flow cases with primary flow only, the surrounding secondary duct and quarl section were removed to provide complete optical access to the primary jet.

Axial velocity profiles for the measured primary stream flows resembled typical profiles for fully developed flow. Examples are shown in Figure 51, where mean and rms axial velocities for cases $\langle 34,0,0 \rangle$ and $\langle 17,0,0 \rangle$ are compared. The profiles are very similar, differing by a scaling factor of 2. Axial velocity profiles in the secondary stream were affected by the swirl number, with swirl tending to flatten the profile. Tangential velocity profiles resembled Rankine vortexes.

The measured rms velocities (both axial and tangential components) across the primary inlet stream for all three levels of V_p agree well with other

Figure 51. Measured and predicted centerline axial velocities for flow cases with a primary inlet stream velocity of 34 m/s.

Figure 52. Comparison of measured and predicted centerline rms velocities for flow case <34,5,0.9>. The predicted axial rms velocity curve is not shown because of its close similarity to the tangential rms velocity curve.

Figure 53. Comparison of LDA data with a PCGC-2 prediction for the axial velocity profile at the 27 cm axial location for flow case <34,0,0>.

Figure 54. Tangential velocity measurements made with the upgraded LDV system the pointed combustor flow case of Jones (1984). Primary and secondary inlet velocities are 13 and 10 m/s, respectively. Secondary air number is 2.

measurements in fully developed pipe flow (Ribeiro and Whitelaw, 1980; Capp, and George, 1982; Martin and Goucat, 1982). Replicate inlet measurements showed no discernible differences in the rms profiles, and where symmetry could be examined (in the primary stream only), it was within 5%. There was some concern that the LDV measurements of rms velocity in regions of steep axial velocity gradients at the inlet might be biased upward because of resolution effects. (If the probe volume extends simultaneously over regions with significantly different mean velocities, the measured rms velocity will be inflated.) However, the agreement of the data with other measurements in flows without resolution problems indicates that adequate resolution was achieved.

PCGC-2 Predictions

Several predictions related to the simulated gasifier cold-flow tests were made with PCGC-2 (Smith, et al., 1981; Smoot and Smith, 1985; Fletcher, 1983), which employs the $k-\epsilon$ turbulence model. In evaluating PCGC-2, predictions of mean and rms velocities were compared with experimental data. Comparisons were made for both centerline values along the axis of the flow chamber and for radial profiles at various axial locations.

In Figure 52, centerline values of axial velocity at various axial locations for several different flow cases are shown. These flow cases all have the same mean primary inlet velocity, 34 m/s. The data show the effects of swirl and secondary stream flow on the centerline axial velocities. Comparisons from case <34,0,0> (primary flow only) with case <34,5,0> (primary flow and unswirled secondary flow) show that the secondary stream decreases the rate of axial velocity decay. The presence of swirl in the secondary stream (case <34,5,0.9>), however, enhances mixing and causes a velocity decay rate greater than when no secondary stream flow is present.

A prediction from PCGC-2 made using standard theoretical inlet boundary conditions (1/7-power law, forced vortex in the secondary duct, eddy diffusivity inversely proportional to a length scale (details are given in Lindsay, 1986) is also shown on Figure 51. The prediction for case <34,5,0.9> shows reasonable agreement with the corresponding data. However, the predictions for the other experimental cases of Figure 51 are virtually the same as the prediction shown. The prediction for case <34,0,0>, for instance, is only 0.7 m/s higher at the 27 cm location than the prediction shown in Figure 51, whereas the data show a difference of nearly 4 m/s at that location. The observed differences between the three experimental cases in the first 30 cm of the flow chamber are consistently much greater than the code predicts. Similar trends were observed for other flow cases. In general, the centerline axial velocity near the inlet is underpredicted, while the axial velocity further downstream (past roughly 30 cm) is overpredicted at the centerline.

In addition to inherent limitations of the $k-\epsilon$ model, other specific factors may hinder the accuracy of the predictions. Errors associated with numerical diffusion (Sturgess and Syed, 1985) and with the limited resolution of the grid structure (40x40 total nodes) are suspected. Both sources of error would be reduced through the use of a finer grid structures. Some of the low-Reynolds number flows of this study are expected to be difficult to predict because the $k-\epsilon$ model assumes steady, high Reynolds number flow. A

correction for low local Reynolds numbers has been developed by Jones and Launder (1972; 1973).

Figure 52 compares measured axial and tangential rms velocities along the chamber centerline for case <34,5,0.9> with the prediction of tangential rms velocity. The prediction agrees well with the measured tangential velocity component. The predicted axial rms velocity curve is not shown because it is nearly the same as the predicted curve shown. While the predicted axial rms values are always higher than the corresponding tangential predictions, the maximum difference is 8% at the peak in Figure 52 and approaches 0% at the inlet and outlet. In the regions where experimental data are available, the predicted rms velocities differ by a maximum of 5%. The measurements show the axial rms velocity component to be consistently about 50% higher than the tangential component. This agrees well with other measurements in related flows (Champagne and Wygnaski, 1970; Capp and George, 1982). The model assumption of isotropic eddy diffusivity does not require the predicted rms velocities to be isotropic, but the predictions for case <34,5,0.9> are nearly isotropic and in this respect do not agree with the data. Similar results were obtained with other flow cases. Some of the difficulty in predicting the differences in rms velocity components is probably due to the current assumption in the code that all local rms velocity components are equal at the inlet plane and at the outlet plane. (This is a consequence of the Boussinesq assumption in fully developed flow. Fully developed flow is assumed at the inlet and at the outlet.) Modified inlet and outlet conditions have therefore been recommended for future predictions to allow more realistic rms velocities to be specified at the inlet and outlet planes. Further evaluation of PCGC-2 is given in Lindsay (1986).

In Figure 53, a PCGC-2 velocity profile is compared with measurements for case <34,0,0> at the 27 cm axial location. Three sets of measurements made on different days have been compiled in this figure. The centerline axial velocity was underpredicted, although some similarities in the observed and predicted profiles are evident.

Measured inlet conditions were used as code input in a number of predictions. Results were then compared to predictions made without the benefit of inlet data. Surprising agreement was found. For instance, superimposed plots of centerline axial velocity predictions for the two types of predictions were often indistinguishable. This is partly because the assumed mean velocity inlet conditions used by PCGC-2 were close to the observed conditions, although that would not always be the case. Predictions were generally insensitive to the specified inlet turbulent intensity (inlet turbulent intensities could differ by a factor of 3 without noticeably affecting predictions beyond the 10 cm axial location). For the flows of this study, therefore, the use of experimental data for the inlet profiles did not appear to improve the accuracy of the predictions, although the data were useful as a check on the a priori inlet computations of PCGC-2.

Simulated Combustor Results

At the completion of the simulated gasifier test series, the inlet of the cold flow facility was modified to simulate the inlet geometry of the laboratory combustor. An axial velocity profile measurement was made in flow conditions similar to those used by Jones, et al. (1984). The measured

profile was similar to the profiles reported by Jones, showing a central recirculation zone pierced by the primary jet. While it has been shown that the tangential velocity profiles reported by Jones, et al. (1984) were distorted due to optical noise, spectral analysis and this repeated combustor measurement suggest that his axial velocity profiles are reliable.

LDV measurements were then made with the two-frequency system. The strongly swirled flow case investigated by Jones, et al. (1984) in the simulated coal combustor was reproduced. The high secondary air flow rate (40 g/s) required re-installation of the Valtek valve system which had been replaced with a gas regulator for the simulated-gasifier test series. The LDV system was used to make tangential velocity measurements in the flow using the weaker blue laser beam (488 nm), the new photomultiplier tube, and the new TSI signal processor as a check on these components. Measurements were then made across the diameter of the chamber at the 41 cm axial location. Tests were made on two different days. Figure 54 shows the tangential velocity results. The flow case has nominal mean primary and secondary velocities of 13 and 10 m/s, respectively, and a secondary swirl number of 2. Some asymmetry in the flow is evident, probably due to the perturbation caused by optical port. Replicate measurements show that the flow is stationary. This was the first successful set of LDV tangential velocity data in the simulated BYU combustor flows.

Conclusions

Measurements of mean and rms axial and tangential velocities were made in 20 cold-flow cases in a simulated entrained gasifier. Unsteady flow regimes were found. Flow transitions (oscillations between metastable states) were associated with the low chamber Reynolds numbers of these flows. Examination of time-averaged results showed that even weak swirl significantly increased the axial velocity decay in the reactor.

Comparison of experimental data with PCGC-2 predictions shows reasonable agreement in some aspects of the predictions, and lack of agreement in others. Centerline axial velocity, for instance, is somewhat underpredicted near the inlet and overpredicted near the outlet. Use of a finer grid structure, improved numerics, and implementation of a low Reynolds number correction to the k- ϵ model may offer improvements in the predictions. Predictions were generally insensitive to the details of the inlet profiles. Use of experimental inlet data did little to improve the accuracy of the predictions for the geometry and flow cases of this study. A two-frequency LDV system was installed and demonstrated. Measurements have been demonstrated in a simulated combustor.

Subtask 1.4 - Advanced Diagnostic Instruments

Background

The eventual introduction of nonintrusive laser diagnostics into the gasifier will allow more precise spatial measurements of temperature and species concentration measurements without the disturbing influence of an intrusive probe. And while the repetition rate of the pulsed lasers is low, ca. 10-20 Hz, some temporal data on the effects of mixing and chemical rate

will also be possible. The objective of this task was to investigate the feasibility of using coherent anti-Stokes Raman spectroscopy (CARS) as a diagnostic tool for probing gasifier flames. Fortunately, a DOE instrumentation grant (DOE Grant No. DE-FG05-84ER75153) was obtained by the Combustion Laboratory to install a CARS system. Consequently, this investigation was broadened to include the development of an instrument for eventual probing of the gasifier.

The assembly of the CARS instrument and an associated laminar flame burner was completed. The CARS instrument is housed in a separate room in the Combustion and Reactions Laboratory Building. This building, which was remodeled by the University for use by the Combustion Laboratory, contains the entrained coal gasifier and the coal-water-mixture combustor. The CARS instrument is housed in the adjacent Optics Laboratory room. It will be possible to pipe the laser beams to the combustion test cells using mirrors, prisms, and lenses in the same manner as is done at the Sandia National Laboratories Coal Combustion Facility in Livermore, California (Hartley and Gusinow, 1981). The signal is to be returned to the spectrometer in the Optics Laboratory by a fiber optic cable. It is necessary to use this type of arrangement because of the rather dusty environment which surrounds the coal reactors and the need to maintain the optical components in a clean environment.

CARS Instrument Design

The CARS instrument in the BYU Combustion Laboratory, shown schematically in Figure 55, has been closely patterned after CARS systems in use at United Technologies Research Center (UTRC) in East Hartford, Connecticut (Stufflebeam, et al., 1983). The source of power for the CARS instrument is a Quanta Ray Nd:YAG laser, operating in pulsed mode at 10 Hertz, whose infrared output at 1064 nm is frequency doubled to 532 nm (green) to form the primary pump beam.

After a careful review of the available dye lasers and their limitations, it was decided to construct two broadband dye lasers patterned after those in use at UTRC (Eckbreth and Anderson, 1985). This dual broadband technique, one of the newest innovations in CARS technology, allows spectra from several gas species to be generated simultaneously.

Prisms are placed in the primary pump beam so that the optical path length of the pump beam can be adjusted to be in phase with that of the oscillator dye beams. Galilean telescopes in the primary pump beam and each of the dye beams are inserted in order to vary the beam waist diameters and to provide some beam steering capability. The primary pump beam then passes through a compound mirror which splits the beam into two parallel beams of equal intensity. The two resulting pump beams and the two dye beams are brought into a three-dimensional and parallel configuration by dichroic mirrors. This configuration, called folded BOXCARS (Shirley, et al., 1980), provides the proper beam phase matching required to effectively generate, and later separate, the CARS signal.

The properly aligned pump and Stokes beams are focussed by a field lens to a point above a small, bench scale burner that is enclosed in a pressure vessel. The burner and associated pressure vessel are located on a traversing

Figure 55. CARS system in the BYU Combustion Laboratory.

mount by which the burner can be moved from side to side or up and down to allow measurements to be taken at different positions above the burner. The point at which the beams intersect is called the diagnostic volume and is the volume in which the CARS signal is generated.

Optical Multi-Channel Analyzer and Spectrometer

Due to the coherent nature and phase matching of the pump and Stokes beams, the CARS signal is laser-like in nature and is generated in a forward direction from the diagnostic volume. After exiting the pressure vessel, the pump, Stokes, and CARS laser beams are collimated by a second field lens. The CARS beam is then separated from the residual pump and Stokes beams by strategically placed apertures and a dichroic mirror, and focussed into a 125 micron diameter fiber optic cable. The CARS signal emerging from the fiber optic cable is taken directly into the homemade spectrometer. An optical multichannel analyzer (OMA) is used as the detector for the spectrometer.

The 0.75 meter, f/3.5 spectrometer was designed to match the speed and resolution of the fiber optic cable (f/3.6) employed for signal transmission in order to optimize coupling efficiency between the spectrometer and fiber optic cable. Inside the spectrometer, a custom holographic grating focusses the CARS signal and resolves it by wavelength onto an EG&G/PARC model 1421 intensified silicon photodiode array. This detector, part of a EG&G/PARC OMA III system, contains 1000 intensified photodiodes (pixels) which detect the signal intensity and which are sequentially read by a detector interface and controller. The spectral resolution of the spectrometer/OMA system has been experimentally determined to be approximately 0.6 cm^{-1} per pixel. This fiber optic/spectrometer/OMA combination, which is similar to those used successfully by UTRC to make diagnostic measurements across the exit of an afterburning turbojet engine exhaust (Eckbreth, et al., 1984), and one used in a portable CARS instrument (Anderson, et al., 1985) worked well.

Data Acquisition Computer and Code

A Digital Equipment Corporation (DEC) MicroVAX II computer is used for the collection and reduction of CARS data. A computer program has been written to interactively send commands to and control the flow of data from the OMA interface. Data are currently being passed through standard RS-232 serial ports, but an OMA 1461/98 High Speed Serial Parallel interface and a DEC DRV11-WA high speed interface to the computer's internal hard disk has also been incorporated into the system. The determination of gas temperature or species concentration with the CARS technique is done by comparison of the experimental spectra with computer generated (theoretical) spectra. The BYU Combustion Laboratory has acquired a computer code from Sandia National Laboratory, Livermore, California, which generates theoretical CARS spectra (Palmer, 1986). The CARS computer code is necessary in order to interpret the measured spectra in terms of temperature and species concentrations.

Bench-Scale Burner and Tests

A small bench-scale laboratory burner capable of operating at high pressure was designed and constructed for use with the CARS system. To date, measurements have been demonstrated in pure gases (e.g. N_2 and CO) at atmospheric pressure conditions, and in $\text{CO}/\text{C}_2\text{H}_4/\text{air}$ flames at atmospheric

pressure. The CARS system has been found to work very well. Workers in the BYU Combustion Laboratory will use the CARS instrument to conduct a series of independently funded experiments in simple bench scale laminar flames at atmospheric and elevated pressure in order to gain experience in use of the instrument. Funds for continuing CARS combustion research in pressurized laminar flames are presently being provided through a NSF grant for an Advanced Combustion Energy Research Center (ACERC) for combustion research at BYU (NSF Cooperative Agreement No. CDR-8522618). It is also planned to incorporate the CARS instrument into the combustion and gasification facilities and make CARS temperature and gas concentration measurements.

III. TASK 2: TWO-DIMENSIONAL COAL GASIFIER MODEL DEVELOPMENT

The purpose of Task 2 was to improve the two-dimensional pulverized coal gasification and combustion model (PCGC-2) and to use the model to describe gasifier processes.

Subtask 2.1 - Physical Submodel Improvement

The purpose of Subtask 2.1 was to review, extend, correlate, incorporate, and improve selected submodels and submodel parameters used in the comprehensive model of coal gasification and combustion.

Coal Devolatilization Model Parameters

The purpose of this investigation was to evaluate devolatilization data and models to determine those appropriate for comprehensive models. Combustion models depend on accurate predictions of devolatilization rates. It is not uncommon for 60% of the mass of a coal particle to combust through devolatilization. Devolatilization models of greatly differing complexity and state of development have been proposed and fitted to experimental data. However, the difference in the modeled devolatilization rates of coals indicated by the different investigators has exceeded several orders of magnitude (compare Kobayashi et al., 1977, and Solomon et al., 1986, at 1400 K for example). Recent work suggests that comprehensive model calculations are more sensitive to devolatilization and oxidation rate parameters than to most other input variables (Smoot and Smith, 1986). Analysis of char oxidation rate parameters is discussed in the next section of the report. Devolatilization rate parameters are discussed in this section of the report and oxidation rate parameters in the following section.

Classical devolatilization data were reexamined to determine appropriate devolatilization parameters for use in comprehensive models and to evaluate the ability of the devolatilization model to correlate data. An optimization computer code, called OPTDES.BYU (Parkinson, et al., 1984), was coupled with a reacting particle model to perform the regression analysis in this study. Generalized reduced gradient (GRG) and sequential quadratic programming (SQP) algorithms were used to perform the regression (optimization) of the models subject to physical constraints.

A reacting particle model was written as part of this study. It is similar in form and philosophy to other particle models which are used at BYU. Care was taken to properly account for the heat and mass transfer effects on particle temperature as the particle reacts. In combustion environments the heat/mass transfer rates are high and can become strongly coupled. This particle model is used to optimize the parameters of the devolatilization submodel.

The flowfields from which the experimental data were gathered were modeled using PCGC-2. Since the particle loadings were light, the effect of changing devolatilization model parameters on the overall flowfield was ignored.

A rigorous statistical analysis of parameters in nonlinear models is discussed in conjunction with the char oxidation study documented in this report. The statistical approach used in this study to determine the parameters for the devolatilization model was similar. Statistical inference about the goodness of fit is also used in the interpretation of the results of this study.

Devolatilization Model. A simple and practical approach to modeling devolatilization was presented by Kobayashi et al. (1977). This model describes devolatilization as the result of two competing chemical reactions, each of which produces a prescribed fraction of coal and volatiles. Mathematically, the model is formulated as

$$C \xrightarrow{k_1} (1-Y_1) S_1 + Y_1 V_1 \quad (7)$$

$$C \xrightarrow{k_2} (1-Y_2) S_2 + Y_2 V_2 \quad (8)$$

$$\frac{dc}{dt} = r_p = -(k_1 + k_2) c \quad (9)$$

$$\frac{dv}{dt} = \frac{dv_1}{dt} + \frac{dv_2}{dt} = r_v = (Y_1 k_1 + Y_2 k_2) c \quad (10)$$

where the reaction rate coefficients, k_1 and k_2 , are given as

$$k_i = A_i \exp(-E_i/RT) \quad i = 1,2 \quad (11)$$

The parameters to be optimized are the preexponential factors, A_1 and A_2 , the activation energies, E_1 and E_2 , and the fractions of volatiles produced from each reaction, Y_1 and Y_2 . In the above equations, C represents raw coal, S represents char (the solid product of coal devolatilization), and V represents the volatiles. The values of Y_1 and Y_2 are between 0 and 1, E_1 is less than E_2 , and Y_1 is less than Y_2 . In practice, Y_1 is often set equal to the volatile yield from proximate analyses. No such constraint was imposed in this study. This is the most commonly used devolatilization submodel in PCGC-2.

Experimental work of Kobayashi. Kobayashi et al. (1977) introduced coal samples into a hot, gaseous, inert environment in a laminar flow furnace (Figure 56). The key features of the system are its axisymmetric geometry, the air preheater for the secondary gases (plasma gun), the coal/cool air feeder, and the heated walls of the muffle tube. Coal was fed from the top and was gathered through a probe at various axial locations in the muffle tube. The percent mass loss was determined from the gathered sample and the residence time of the particle was determined by the particle velocity and distance to the collector. Mean gas temperatures varied from 1000 K to 2100 K, and the gas velocity in the reactor varied from 0.81 m/s to 8.65 m/s. The reactor has a 50.8 mm I.D. and the distance from the coal injection tube to

Figure 56. Reactor used in the experimental work of Kobayashi et al. (1977).

the collection probe varied from 0.01 to 0.22 m. Simple corrections for nonisotropic sampling were made. Figure 57 illustrates the resulting mass loss data for a bituminous coal entrained in gases at six different temperatures. The lines in the figure represent a correlation of this data which is discussed later.

Flowfield Model. The temperature, velocity, and radiation conditions within the reactor were modeled with PCGC-2, (Smoot and Smith, 1985). Results of the axial velocity and temperature predictions for the 2100 K case are illustrated in Figures 58 and 59. The contour plots of these figures are oriented with flow going from left to right. The bottom of the contour plot is the reactor centerline and the top is the reactor wall.

Particle Reaction Model. The particle model predicted the particle response to the flow data predicted by PCGC-2. The heat transfer rate between the assumed spherical particle and the gas is

$$q_p = \theta k T_p A (T_g - T_p) + r_v \int_{T_p}^{T_g} C_p dT + q_{ra} + q_{rx} \quad (12)$$

where the first term represents the heat being convected/conducted to the particle, the second term is the sensible heat required to raise the mass evolving from the particle to the surrounding temperature, the third term is the radiative heat transfer, and the last term accounts for heats of reaction in the particle. The heats of reaction of the devolatilization reactions are very small and were neglected in this study.

The first factor of the first term on the right hand side of Equation 12 is a blowing parameter and represents the effect which mass transfer has on the ability of heat to transfer to the particle. This parameter represents the major source of coupling between the heat and mass transfer rates.

The particle mass balance, as given in Equations 7-11, and the particle momentum equation were solved simultaneously with the heat transfer equation. The particle momentum equation was solved by standard techniques (Bird et al., 1966). A predictor corrector algorithm was written to solve the simultaneous equations. Figure 60 is representative of the predicted results from the integration of the particle reaction scheme, predictor corrector solution technique, and flow field data from PCGC-2.

This figure illustrates the magnitude of the impact which mass transfer rates can have on heat transfer. The temperature of the particle is a complex function of time. The imposed ambient temperature in this prediction was 2100 K. The particle was assumed to have a 100 micron diameter. The plateau observed in the figure between 6 and 11 ms for the constant heat capacity assumption and 8 and 14 ms for the variable heat capacity assumption results from a high rate of mass transfer. The significance of the heat capacity assumptions is discussed later.

The third term, which accounts for the radiative heat transfer from the particle to the gas, is modeled by a flux method (Smith, et al., 1985).

Figure 57. Predictions and data of Kobayashi, et al. (1977) for bituminous coal.

Figure 58. Contour plot and three dimensional projection of axial velocity field in the reactor at 2100 K.

Figure 59. Temperature contours and three dimensional projections for the reactor at 2100 K.

These flux fields were predicted with the temperature and velocity fields by PCGC-2.

Particle Heat Capacity. The devolatilization rates depend on both particle temperature and particle heating rate. The temperature of the particle can be predicted from fundamentally derived correlations if the ambient environment is known. However, the temperature and composition dependence of the particle heat capacity, which is often ignored, must be carefully modeled. Merrick (1983) suggested the following function for the heat capacity of coal.

$$c_v = (R/a) [g_1 (380/T) + 2g_1 (1800/T)] \quad (13)$$

where R is the universal gas constant (8314.4 J/kg-mol/K), a is the average atomic weight of the coal or char (kg/kg-mol), T is temperature (K) and g_1 is the following function.

$$g_1(z) = \frac{e^z}{[(e^z - 1)/z]^2} \quad (14)$$

The constant volume and constant pressure heat capacities were assumed equal in this study. The average atomic weight of the coal, a, is determined by the following equation

$$\frac{1}{a} = \sum_i^n y_i / \mu_i \quad (15)$$

where y is the mass fraction of element i, μ is the atomic weight of element i, and n is the number of elements in the organic portion of the coal. Merrick compared his heat capacity model with data and found agreement within about 10% in the temperature range of 0-300°C and coal ranks ranging from 15-35% volatile matter. Graphite and char heat capacities were correlated within 5% between 0 and 800°C. An initial coal particle diameter of 100 microns was assumed. The dry ash-free (daf) ultimate analysis of the coal was used in this study to determine a = 8.18 for the coal and a = 12.0 for the char, the latter based on a predominate carbon content of the char. The heat capacity of ash was taken to be

$$c_a = 593.3 + 0.586T \quad (T \text{ in K}) \quad (16)$$

after Merrick's suggestion.

Computations were illustrated in Figure 60. The temperatures of both particles rise about 1.6×10^5 K/s initially. Between 0 and about 5 ms the rate of temperature increase of the particle with constant heat capacity decreases because of the diminishing difference between the particle and gas temperatures. Between 5 and 10 ms the particle is predicted to undergo devolatilization, which further inhibits the particle temperature rise. This

Figure 60. Variations of (a) particle temperature and (b) mass loss when different particle heat capacity formulations are used. The variable C_p case uses the correlation of Merrick (1983).

effect was similarly predicted by Ubhayakar and coworkers (Ubhayakar et al., 1977). After devolatilization the temperature of the less massive particle approaches a steady-state temperature. This final temperature is less than the gas temperature due to radiative heat losses to the walls of the reactor. Oxidation rates were arbitrarily neglected in these predictions to more clearly illustrate effects of different heat capacity assumptions.

The temperature history of a particle with variable heat capacity is also illustrated by this figure. All of the effects noted for the constant heat capacity particle are qualitatively observed for the variable heat capacity assumption. The additional effect of heat capacity varying with extent of reaction and temperature significantly slows the rate of particle temperature rise at all stages of the combustion process. The time required to complete devolatilization is predicted to increase by about 50%. At 12 ms, the difference in predicted particle temperatures reaches its maximum of about 500 K. And the time required to reach the steady-state temperature increases by about 70%.

The impact of the different predicted temperatures of the particles on the devolatilization rate is potentially substantial. For example, the 500 degree difference in particle temperature shown in the figure corresponds to a predicted devolatilization rate difference of one to three orders of magnitude, depending on the rate constants used. In addition, the time required to initiate and complete devolatilization is sensitive to this assumption, as illustrated in Figure 60b.

Devolatilization models which are sensitive to heat-up rates, as is the one employed here, will predict different volatile yields for the two assumptions. The volatiles are also predicted to be released at a slightly lower rate and temperature for the variable heat capacity model. These results indicate that temperature and composition dependence of particle heat capacity can significantly affect predicted particle temperature histories and therefore the rate coefficients derived from devolatilization data.

Results and Discussion. Figure 57 illustrated the agreement obtained with the optimized coefficients of the devolatilization model. The measured weight loss of the coal particles can be predicted with good accuracy with the simple two-step model. The figure contains the data for the bituminous coal and a constant heat capacity assumption. The predictions were made using the same set of coefficients for all heating rates. A statistical analysis of the goodness of fit of the correlation of the data in Figure 57 indicates that the data are predicted within their inherent error bounds. The inherent error was estimated from the several near replications in the data points.

The ability of the relatively simple two-step devolatilization model to correlate the weight loss data within its inherent error suggests that the form of this model is adequate to predict the weight loss during devolatilization. This can be done with a single set of parameters for a given coal type over a wide range of heating rates. The variation of ultimate devolatilization yield with heating rate/ultimate temperature is also accurately predicted. One conclusion from this study is that the two-step model is capable of correlating this devolatilization weight loss data within the inherent error.

Suggested coefficients from several coal types and several investigators have been collected and are reported in Table 16, which is also included in Volume II of this report. All of these coefficients are applicable to devolatilization models in PCGC-2 and are expressed in the units appropriate for PCGC-2. The rate coefficients shown in this table indicate a difference in predicted devolatilization mass loss rate of several orders of magnitude. Those investigators which distinguished between the rates for different coal types show comparatively small variations with coal type as opposed to the difference among the results of different investigators. The data enclosed within parentheses was estimated from the referenced articles. In the case of the single step reaction, the ultimate yield (Y) is considered a model parameter which varies with both coal type and heating rate. One important conclusion from this work is that the two-step model is capable of predicting the volatile yield of a given coal over all heating rates of practical interest within the inherent error of the data. It is viewed as substantially superior to the single step models. That is, the values of Y_1 and Y_2 should not need to be altered with changing reactor conditions, but only with coal type.

Based on this work, approximate optimized coefficients for the data of Kobayashi are given below in Table 17.

TABLE 17
OPTIMIZED DEVOLATILIZATION COEFFICIENTS FOR TWO COAL
TYPES ON THE DATA OF KOBAYASHI, ET AL. (1977)

	Constant C_p		Merrick C_p	
	<u>Lignite</u>	<u>Bituminous</u>	<u>Lignite</u>	<u>Bituminous</u>
Y_1	0.47	0.56	0.50	0.60
E_1 (J/kmol)	4.9×10^7	9.02×10^7	3.62×10^7	3.11×10^7
A_1 (s^{-1})	5.8×10^2	1.9×10^4	1.2×10^4	4.3×10^5
Y_2	0.6	0.8	0.62	0.80
E_2 (J/kmol)	2.04×10^8	3.09×10^8	1.91×10^8	2.91×10^8
A_2 (s^{-1})	6.6×10^7	9.7×10^9	2.2×10^9	2.4×10^{11}

These coefficients, and their indicated rates, are quite different, both from each other and from the coefficients originally proposed by Kobayashi. Nevertheless, they resulted in a fit to the data that is within its experimental error for all six heating rates. Kobayashi mentioned that the parameters he suggested were not carefully determined. His correlations did not perform as well under all the heating conditions.

A more detailed explanation of the flow conditions and techniques used in gathering the data used in this study has recently been obtained. The flow rates of the coal carrier gas into the reactor and the particle velocities are somewhat different than had been inferred from the published literature. The

TABLE 16

DEVOLATILIZATION RATE EXPRESSIONS AND PARAMETERS FOR USE IN PCGC-2

Single Step Reactions

Rank	Reference	ω_c^0 (DAF) ⁺	ω_h^0 (DAF) ⁺	Y	A (s ⁻¹)	E (J/kmol)
Lignite	Solomon, et al., 1986	(0.4)	$1 - \omega_i^0$	1.0	4.3×10^{14}	2.29×10^8
	Kobayashi, et al., 1977	(0.7)	"	"	6.6×10^4	1.05×10^8
	Anthony, et al., 1976	(0.4)	"	"	2.83×10^2	4.64×10^7
	Truelove & Jamaluddin, 1986	(0.4)	"	"	6.2×10^3	4.64×10^7
Bituminous	Solomon, et al., 1986	(0.4)	$1 - \omega_i^0$	1.0	4.3×10^{14}	2.29×10^8
	Kobayashi, et al., 1977	(0.7)	"	"	6.6×10^4	1.05×10^8
	Anthony, et al., 1976	(0.4)	"	"	7.1×10^2	4.94×10^7
	Truelove & Jamaluddin, 1986	(0.4)	"	"	2.0×10^4	4.94×10^7
	Wiser, et al., 1964	(0.5)	"	"	4.8×10^1	6.27×10^7
	Badzioch & Hawksley, 1970	(0.4)	"	"	1.14×10^5	7.45×10^7
	Badzioch & Hawksley, 1970	(0.4)	"	"	3.12×10^5	7.45×10^7

Two Step Model

Rank	Reference	Reaction	ω_c^0 (DAF)	ω_h^0 (DAF)	Y _i	A _i (s ⁻¹)	E _i (J/kmol)
Lignite	Kobayashi, et al., 1977	1	1.0	$1 - \omega_i^0$	0.3	2.0×10^5	1.05×10^8
		2	"	"	1.0	1.3×10^7	1.67×10^8
Bituminous	Kobayashi, et al., 1977	1	"	"	0.3	2.0×10^5	1.05×10^8
		2	"	"	1.0	1.3×10^7	1.67×10^8
	*Ubhayakar, et al., 1977	1	"	"	0.4	3.7×10^5	7.36×10^7
		2	"	"	0.8	1.5×10^{13}	2.51×10^8

*Most commonly used parameters if no data are available.

⁺These parameters are expected to vary with heat-up rate and/or temperature.

optimization of the coefficients in this study is being redone under separate funding to assess the impact of these changes.

Char Oxidation Model

The purpose of this task was to evaluate and recommend parameters which are appropriate for char gasification and oxidation rate models. The results are organized into five subsections. The first subsection briefly discusses some statistical concepts which were developed and employed in this study. The second through fourth subsections discuss and illustrate the application of these techniques. The fifth subsection presents the recommended values for the parameters in the rate expressions.

Statistical Treatment of Arrhenius Data. The method to be discussed for parameter estimation for Arrhenius-type data differs from the more common approach of linearization followed by linear-least-squares analysis. This section presents the theory for the nonlinear method and explores the statistical differences between the two methods. Methods for statistical analyses and inference from the results are also presented to determine probable values and confidence contours for the results.

The root of the differences between the methods of data analysis lies in the assumptions about the data. A reasonable assumption is that the data follow an Arrhenius form of an equation with errors in measured reactivity which are normally distributed with a mean of zero and constant variance. The equation for the data in such a case is;

$$k_i = A \exp (-E/RT_i) + \epsilon_i \quad (17)$$

where ϵ_i is the error term.

Equation 17 is not the same as the implicitly assumed form of the error term when the linearized form of the equation is used. The latter equation is shown as Equation 18.

$$\ln k_i = \ln A' - E'/(RT_i) + \epsilon'_i \quad (18)$$

where ϵ'_i has the same definition as ϵ_i . Clearly, the two equations are not equivalent. Several principles of statistical theory indicate that the former, or some generalization of it, is the appropriate equation to use in the analysis of reactivity data. These principles are discussed by Baxter (1987) and are summarized here. A combination of the statistical technique of maximum likelihood estimation, and the central limit theorem, indicates that good estimates of the activation energy and preexponential factor from Arrhenius-type data come from

$$\min_{\text{wrt } A, E} \sum_i^n \left[\left(\frac{\hat{k}_i - k_i}{\sigma_{k_i}} \right)^2 - 2\rho_i \left(\frac{\hat{k}_i - k_i}{\sigma_{k_i}} \right) \left(\frac{\hat{T}_i - T_i}{\sigma_{T_i}} \right) + \left(\frac{\hat{T}_i - T_i}{\sigma_{T_i}} \right)^2 \right] \quad (19)$$

subject to a pointwise constraint of

$$\min_{\text{wrt } k_j, \hat{T}_i} \left[\left(\frac{k_i - \hat{k}_i}{\sigma_{k_i}} \right)^2 - 2\rho_i \left(\frac{k_i - \hat{k}_i}{\sigma_{k_i}} \right) \left(\frac{T_i - \hat{T}_i}{\sigma_{T_i}} \right) + \left(\frac{T_i - \hat{T}_i}{\sigma_{T_i}} \right)^2 \right] \quad i=1, \dots, n \quad (20)$$

The estimates produced by these minimizations appropriately deal with data which are subject to errors in either reactivity or temperature or both, data which have linearly correlated errors in reactivity and temperature, and data with precision which is not constant over their range. The minimizations appropriately reduce to weighted least squares and nonlinear least squares criterion when the assumptions required for these methods are met. In the terminology of statisticians, the parameters produced by the minimizations can also be shown to be unique, consistent, invariant, sufficient, and efficient in all cases where such properties are possible to achieve. The parameters from the linearization technique are unique, but have none of the other properties. In short, the parameters determined from a nonlinear analysis are improved in every theoretical way from those determined from the linear analysis. The remainder of this section illustrates the magnitude of the difference between the approaches and the practical evidence of the theoretical improvements.

Application of Nonlinear Analysis of Arrhenius Data. The improved fit of the nonlinear technique is apparent both in the statistics and in the visual comparison of the data with the correlation lines. Figure 61 illustrates these points. The linear technique comes closer to the lowest temperature data point at the cost of a poorer fit of the rest of the data. The data in this figure are for CO₂ oxidation of a Texas lignite char and were collected by Combustion Engineering (Goetz et al., 1982)]

A statistical comparison of the fit of the two lines shown in Figure 61 shows, with 90% confidence, that the improvement in the fit is significant. Indeed, a statistical analysis of the linear correlation concludes, with over 90% confidence, that the Arrhenius equation does not correlate this data within its inherent error. This would indicate that some more sophisticated model is required to correlate the data. The same test applied to the nonlinear correlation indicates that the lack of fit is not significantly greater than the inherent error in the data. These opposed findings illustrate the erroneous conclusions which can be drawn from the linear fitting technique. The confidence levels cited here and elsewhere in this report should be regarded as approximate because the lack of fit statistic may be biased. The tests and methods themselves are exact, however. The first conclusion from this study is that the improved coefficients can significantly increase the accuracy of correlation within the range of the data.

The gasification rate of chars by CO₂ is practically important at temperatures higher than the highest data indicated in Figure 61. The inset in Figure 61 illustrates the difference in the extrapolated gasification rate for these chars. A lack of data at such high temperatures often forces extrapolation of low temperature data. The difference in the extrapolated reaction rate is substantial and, while extrapolation is prone to error under any circumstance, the extrapolation using the nonlinear parameters statistically is more sound. A practical illustration of this point is

Figure 61. Comparison of linear and nonlinear correlations of kinetic data. Data from (Goetz et al., 1982).

discussed later in conjunction with the work of Field (1969). A second conclusion from this study is that the improved coefficients can have a large impact in the predictions outside the range of the data.

Confidence Intervals (Contours) for the Parameters. The most accurate method of representing the confidence intervals for the parameters is with a contour graph. The theory of producing these contours differs from techniques commonly used in analyzing linear equations and is discussed by Baxter (1987). Typical results are shown here with char oxidation data reviewed by Field (Field et al., 1967) used as an illustration. These data also play a role in the following section of the report. Identical techniques have been applied to gasification data. Field surveyed a large number of investigators and selected work from six of them which provided information on oxidation rates which was free of diffusion limitations and otherwise useful. Parameters were suggested for use in Arrhenius expressions for char oxidation based on a linear analysis of the data.

Using the nonlinear method, the data tabulated by Field were reanalyzed. Figure 62 illustrates the results of this analysis. The point indicated by the circle in the figure is the best estimate of the parameters of the model. The loops in the figure are contours of 50% and 95% confidence for the parameters of the model. That is, the actual parameters for the model have a 50% and 95% likelihood of lying within the respective loops. The preexponential factor varies over a much larger interval than the activation energy, as is expected.

The shape of the loops in Figure 62 indicates that specifying only the endpoints of the confidence contours is a misrepresentation of the uncertainty in the parameters. That is, while the 95% confidence interval is 17 to 28 kcal/mol for the activation energy and 20 and 600 g/(cm²-s-atm) for the pre-exponential factor, there is a vanishingly small probability that one of them would be at its upper bound while the other is at its lower. The contours illustrate this point accurately.

The inset in Figure 62 illustrates the same loops on a scale which includes the best estimate of the parameters from the less rigorous linear analysis. This point lies well outside of the 95% or even 99.9% confidence contour (the latter is not shown), indicating that it is a quite poor approximation to the actual parameters.

The general shape of the contours is a property of the Arrhenius expression. However, the size and detailed shape of the contours depends on the accuracy and number of data. With fewer and less accurate data, the importance of performing a proper confidence contour analysis becomes more pronounced.

The parameters generated by the linearization of the data not only are shown to be poor estimates of the actual best estimates, but can be concluded to not represent the data with a confidence level in excess of 99.9%. Just as in the previous section, where an analysis of the fit of the Arrhenius expression not only improved but actually reversed the conclusion of the statistical test, here the conclusions about the parameters are reversed. The predicted confidence contours also reasonably represent the range of parameters typically measured for char oxidation. A third conclusion of this study, is

Figure 62. Confidence contours for preexponential factor and activation energy based on data from Field et al. (1967). The linear estimate is also shown in the inset.

that the coefficients determined by the common linearization technique can be in large disagreement with more rigorous parameters.

Practical Usefulness of Rigorous Analysis. Data and conclusions which Field published after his above-cited review were used to illustrate the practical usefulness of nonlinear data analysis (Field, 1969). Figure 63 illustrates data collected by Field after his review. These data span a greater temperature range than did the data in Field's review. The lines on the plot are predictions based on the independent data in the review. The predictions based on the linearization analysis are poor. Low temperature reactivities are slightly underpredicted and high temperature reactivities are greatly overpredicted. Field observed this same result and chose to fit his data with a reactivity which is linear in temperature, even though negative reactivities were predicted at temperatures below about 1300 K.

The prediction from the nonlinear analysis of the data is also indicated in the figure. Although a slightly better fit could be expected if the data in the figure were used to determine the correlation, the prediction with the coefficients from the nonlinear analysis accurately represents the data. This illustrates both the improvement in the coefficients and the greater accuracy in extrapolation of the results. A fourth conclusion from this study, is that the improved coefficients can lead to more accurate extrapolation and can explain previously unexplained differences in char reactivity.

These results show how the classical linearization procedure can lead to several poor results. The Arrhenius form of the equation is unjustifiably rejected, the parameters are not justified by the data, and the extrapolation is poor. However, a proper statistical analysis indicates a great deal more consistency and accuracy in the data than have previously been reported.

Coal Gasification and Oxidation Data. The techniques above apply to any type of correlating expression for data. However, current research seldom extends beyond Arrhenius expressions for either global or intrinsic reactivity. Several authors have suggested that Langmuir-Hinshelwood expressions, which account for effects of adsorbed species, are more appropriate (see Smoot and Pratt, 1979 for a discussion, Muehlen, et al., 1981, for a good example of data). The coefficients which are required for these expressions are ill defined and will require more fundamental research before the expressions are useful. Coefficients for global kinetics were gathered in this study.

Several sets of data for the oxidation rate of various coals are available. Table 18 lists coefficients suggested by several investigators. Wherever possible, the data were reanalyzed according to the preceding methods. The results from the reanalysis are also listed in Table 18 and are referred to in Baxter (1987). The differences are often substantial. The coefficients designated with an asterisk are viewed as most accurate for use in the code if data for a specific case are not available.

Data for the gasification rate of coal (i.e., reactions with CO_2 and H_2O) are rare. None were found which were of the same quality as the oxidation data marked by asterisks. Nevertheless, coefficients based on the scarce existing data are also listed in Table 18. Coefficients from both the linear and nonlinear analysis are also indicated here. These data sets often contain outliers, that is, a number of points which substantially disagree with the

Figure 63. Comparison of accuracy of extrapolation and comparison of experimental results between reviewed work of Field et al. (1967) and data of Field (1969).

TABLE 18

KINETIC RATE PARAMETERS FOR CHAR REACTION WITH O₂, CO₂, AND H₂O

$$\frac{d\alpha_n}{dt} = AT_{\text{exp}}^n (-E/RT) [\text{oxidizer}]$$

Oxidizer	Rank	Reference	n	A (m/K ⁿ s)	E (J/kmol)		
O ₂	*	all ranks	Baxter, 1987	1.0	2.30	9.29 x 10 ⁷	
		all ranks	Field, et. al., 1967	1.0	0.30	1.49 x 10 ⁸	
		h _v Bituminous A	Baxter, 1987	1.0	1.03	7.49 x 10 ⁷	
		h _v Bituminous C	"	1.0	0.479	5.25 x 10 ⁷	
		Subbituminous C	"	1.0	10.4	9.31 x 10 ⁷	
		h _v Bituminous A	Goetz, et. al., 1982	1.0	2.25	8.52 x 10 ⁷	
		h _v Bituminous C	"	1.0	2.02	7.18 x 10 ⁷	
		Subbituminous C	"	1.0	4.96	8.36 x 10 ⁷	
	CO ₂		Lignite	Baxter, 1987	1.0	3.419	1.30 x 10 ⁸
			h _v Bituminous A	"	1.0	1160.0	2.59. x 10 ⁸
		h _v Bituminous C	"	1.0	4890.0	2.60 x 10 ⁸	
		Subbituminous C	"	1.0	6188.0	2.40 x 10 ⁸	
		Lignite	Goetz, et al., 1982	1.0	45.0	1.65 x 10 ⁸	
		h _v Bituminous A	"	1.0	95.14	2.25 x 10 ⁸	
		h _v Bituminous C	"	1.0	88.5	2.36 x 10 ⁸	
		Subbituminous C	"	1.0	70.95	1.78 x 10 ⁸	
		Graphite	Mayers, 1934	1.0	4.40	1.62 x 10 ⁸	
H ₂ O			Graphite	Mayers, 1934	1.0	1.33	1.47 x 10 ⁸
		Lignite	Otto, et al., 1979	1.0	4.26 x 10 ⁴	3.16 x 10 ⁸	
		Lignite	"	1.0	208	2.40 x 10 ⁸	

*Recommended good estimate if no data are available.

general trend of the rest of the data. In some cases, the outliers have a large effect on the predicted coefficients.

Turbulent Particle Dispersion

The purpose of this task was to review and revise the current formulation of the turbulent particle dispersion submodel.

Review of Current Model. The original particle dispersion submodel in PCGC-2 derived its form from a heuristic analogy between the impact of turbulent eddies on particles and molecular diffusion processes. A Fickian diffusion process was postulated for the dispersing effect of turbulence on particles. The functional form of the diffusion coefficient depended on particle diameter and turbulent intensity according to

$$k_p = A \epsilon_g (1 + t_p/t^t)^{-1} \quad (21)$$

where k_p is the particle mass diffusivity, A is a global constant, ϵ_g is the gas momentum eddy diffusivity, and t_p and t^t are particle and turbulence relaxation times. Such a diffusivity depends on particle diameter and turbulent intensity in a logical way. This definition, combined with some empirically determined global parameters, has been reasonably accurate in many cases in the past. Smith and Baxter (1986) reviewed this performance in a paper published during this contract. A review of the theoretical bases for the model is conducted by Baxter (1987). However, occasionally the current model leads to physically unrealistic results and the theoretical bases are not always sound. Therefore, a more rigorous theory has been developed.

Improved Particle Dispersion Submodel. The theory of an improved particle dispersion submodel is derived and critically examined by Baxter (1987). It is based on Taylor's theorem from turbulence theory, stochastic process modeling, and several results from Ito's calculus (a calculus which deals with randomly varying functions). Within the assumptions discussed in the derivation, the most important resulting equations are

$$P(x,y,z) = \frac{q}{(2\pi)^{3/2}} \int_0^t \frac{1}{\sigma_x \sigma_y \sigma_z} \exp \left(- \frac{(x-\bar{x})^2}{2\sigma_x^2} - \frac{(y-\bar{y})^2}{2\sigma_y^2} - \frac{(z-\bar{z})^2}{2\sigma_z^2} \right) dt' \quad (22)$$

where

$$\sigma_i^2 = 2 u'^2 \int_0^t \int_0^{t'} R(\tau) d\tau dt' \quad i = x,y,z \quad (23)$$

P is a multidimensional probability density function for particle position, and σ_i^2 is a variance in position for each coordinate direction. $R_p(\tau)$ is the Lagrangian autocorrelation function for the particles.

This approach to turbulent particle dispersion is a first principles solution to the extent that the autocorrelation function is known. Fundamental solutions to Equation 22 are known which make this approach exact in each of the limits of no turbulence, homogeneous turbulence with uniform mean flow, Brownian particles, and large particles. Approximate functional forms for the autocorrelation function $R_p(\tau)$ are known for particles which track the gas exactly.

This theory is the foundation of a more fundamental turbulent particle dispersion submodel which is entirely Lagrangian in its formulation. A small number (10-150) of representative trajectories are computed to simulate the overall particle field, as in the past. The particle number density field is based on the probability density function as in, Equation 22. The variances in the probability density function are calculated according to Equation 23. Particle number densities are computed from the overall flowrate of particles and the probability density function. The number density fields are used to weight the particle source terms in the Eulerian computational cells for a distance of three standard deviations in all coordinate directions from the mean particle position. Although all of the source terms will be calculated at any given time by the Gaussian probability density function (Eqn. 22), the final source terms and number densities will not be proportional to each other, or even Gaussian, in general. The source terms depend on instantaneous rates of reaction and flow patterns, both of which can make them non-Gaussian.

This submodel explicitly allows for multidimensional effects in the calculations of both the mean trajectories and their variances. Appropriate modifications can be made in the case of correlated fluctuations. However, predicting such correlations is outside of the scope of most turbulence models.

This model also predicts Eulerian particle information with more accuracy and generality than the previous model. For example, average particle diameter, temperature, composition, etc. are stored at each Eulerian computational cell along with the source terms for the Eulerian equations. These particle properties should enhance the accuracy of the Eulerian calculations which depend on particle properties (radiation, for example). The variations in particle source terms from cell to cell are smooth, allowing for the calculation of their gradients and possible improvements in turbulence modelling of reacting flows. The distribution of source terms should also decrease the number of required particle simulations and increase the stability of the iterations between particle and gas phase calculations. These advantages could also reduce the computational time required to converge a case.

Status of Submodel Development. This turbulent particle dispersion submodel has been coded as an independent model, requiring the turbulence properties of the gas phase to be specified. The results of this calculation have been compared to other models and analytical results. Figure 64 illustrates one such comparison. Both of the results for the stochastic flow models illustrated in the figure were predicted by Shuen et al. (1983). The difference was an arbitrary change in the time constant used to characterize the turbulent flow, the actual value being taken from the source cited in the figure for each case. These are compared with an analytical solution by Hinze (1975). The analytical solution and the stochastic flow solutions assumed a

Figure 64. Comparison of previous turbulent particle dispersion models and model developed under this contract with analytical results. Figure adopted from Shuen et al., 1983.

constant eddy diffusivity for the particles. Under these assumptions, this model predicts the analytical solution exactly, as illustrated.

The stochastic flow models typically require over 2000 particle trajectory calculations for each particle size/type and each starting location to produce one result similar to that shown in Figure 64. This new model required one particle simulation. In practical applications, the simulation requires about twice as long to compute as a single particle trajectory calculation in the stochastic models because of the required integrations under the probability density function. Therefore, the model is approximately three orders of magnitude more efficient than the stochastic flow model, and can yield results that are more accurate.

The analytical solution in Figure 64 required the assumption of a constant eddy diffusivity. This assumption is useful for these kinds of comparisons, but is rarely valid in flows of practical interest. Figure 65 illustrates the ability of the model to predict the change in diffusivity with time. The differences in the solutions are never greater than about 1% and these are due to numerical and roundoff errors. The curvature of the predicted lines indicates that the diffusivity, which is proportional to the variance divided by the time, is not constant. Although the variation in diffusivity was arbitrarily chosen in this case, it is representative of actual turbulent dispersion data, as illustrated in Figure 66. The data in this figure are for the lateral dispersion of hydrocarbon droplets in turbulent flow. The flow was fully developed and steady, so the normalized distance is proportional to a normalized time.

The scope of problems for which there are analytical solutions is represented by these comparisons. The new model is designed such that it yields the analytical solution (within roundoff and numerical error) in all cases where one exists. Flows of practical interest to coal combustion and gasification and turbulent particle dispersion for 50-150 micron particles generally do not have analytical solutions. The results of these idealized comparisons are encouraging from both computational and theoretical viewpoints. Therefore, under separate funding the independent submodel developed under this contract is being incorporated into PCGC-2 for further comparison to data and future use.

Subtask 2.2 - Numerical Solution Efficiency

While numerical solutions to computer combustion systems have been possible for several years, considerable effort is presently being made to reduce the computational costs. The objective of these efforts is to make the amount of computational work proportional to the amount of real physical changes in the computed system (Brandt, 1984).

General Convergence of PCGC-2

Figure 67 shows the convergence pattern for a typical PCGC-2 simulation. Though the definition of convergence is somewhat arbitrary, convergence has not been obtained after the initial 20% of the iterations. Thus we see that considerable computational time is being expended for small, but necessary, changes. This phenomenon of requiring large amounts of work to

Figure 65. Analytical and modeled solutions to turbulent particle dispersion in which the effective diffusivity is not constant.

Figure 66. Experimental turbulent particle dispersion data which exhibits behavior similar to Figure 65. Data from Kalinske and Pren, 1944. Figure adopted from Hinze, 1975.

resolve small changes is called numerical stiffness. Brandt (1984) has recently attributed numerical stiffness to the existence of several solution components with different scales, which conflict with each other.

Figure 68 shows the convergence pattern of an individual node in the computational field, for axial velocity, for two cases with different grid resolutions. (In each case, the node was at the same physical location in the reactor). The final values of axial velocity differ (due to grid resolution) and the patterns in which the errors are reduced also differ. Figure 69 illustrates the overall convergence pattern for axial velocity. In each of the four frames, the solution at some 'computational time' is compared with the converged solution. A 'rolling' type pattern is evident, proceeding from the front of the reactor towards the exit. This type of phenomenon occurs, regardless of the resolution of the grid. These two figures illustrate the existence of different solution components, with different scales, that must be resolved.

Approach

Most of the numerical stiffness exhibited by PCGC-2 is in the fluid-dynamics model. It was decided to limit the efforts in this study to the fluid-dynamics sub-model. A simplified version of PCGC-2, called MAXIGAS, was generated for these investigations. For more detail concerning MAXIGAS, see (Hedman, et al., 1985). Four different techniques or approaches investigated to improve the numerical efficiency (or reduce the numerical stiffness) of PCGC-2 were: 1) under-relaxation factors, 2) adaptive grid techniques, 3) multigrid techniques, and 4) new techniques to couple momentum and continuity equations.

Under Relaxation Factors. Under-relaxation is necessary to maintain the numerical stability of SIMPLE/SIMPLER techniques. Under-relaxation reduces the magnitude that a variable can change between two iterations. A variable is under-relaxed, because both large changes will make that particular calculation unstable and because of its effect on the other variable calculations. For greatest efficiency, the largest possible value of an under-relaxation parameter, which still maintains stability, should be used. The most common usage of under-relaxation factors is to find one value for each variable, and use that value for the entire computation. The investigations in this area centered on attempting to adjust the under-relaxation factors both temporally and spatially. As the computations progress, and convergence is approached, the amount that a variable is changing between any two iterations will be reduced. Thus, higher values of under-relaxation factors should be able to be used. Furthermore, different parts of the computational domain converge at different rates. Spatial optimization of under-relaxation factors should also help numerical efficiency.

Several different techniques of under-relaxation were investigated, including under-relaxing each variable sequentially at each node

$$\phi_p^{i+1} = r\phi_p^{i+1} + (1-r)\phi_p^i \quad (24)$$

Figure 67. Rate of convergence for axial velocity.

Figure 68. Axial velocity predictions and respective errors for two different grid distributions. The location of these predictions, in the computational domain, remained constant for both cases.

a. 15 iterations

b. 30 iterations

c. 45 iterations

d. 60 iterations

Figure 69. Comparisons of three-dimensional axial velocity projections at incremental times with the converged projection (74 iterations).

and under-relaxing the coefficients and source terms (simultaneous under-relaxation) (Fiveland, 1984),

$$C_p' \phi_p^{i+1} = \sum C_{NB} \phi_{NB} + S' \quad (25)$$

where $C_p' = C_p / r$ and $S' = S + \frac{(1-r) C_p \phi_p^{old}}{r}$

The latter has always been used by PCGC-2 (and MAXIGAS). Also, various inertial under-relaxation schemes were examined (Patankar, 1980).

$$(C_p + I) \phi_p^{i+1} = \sum C_{NB} \phi_{NB} + S + I \phi_p^i \quad (26)$$

Of particular interest was a very rigorous inertial under-relaxation technique developed by Neuberger, et al., (1983) that adjusts the under-relaxation factors both temporally and spatially. They demonstrated some impressive improvements in the efficiency of turbulent fluid flow computations made with SIMPLE. Unfortunately, after a significant effort, these improvements could not be reproduced in MAXIGAS.

The conclusion made after evaluating each of the above techniques is that the method currently employed by PCGC-2 is the most efficient. Lilley and Rhode, (1982) use this same method and vary the global under-relaxation values based on iteration number. This and similar approaches are not thought to be acceptable for PCGC-2 because of the wide range of systems (wide range of convergence patterns) that this code attempts to predict. However, a algorithm to adjust the global under-relaxation factors based on the value of the greatest normalized residual has been successfully incorporated into MAXIGAS. At best, this method reduces computational time by 10%, and does not further address numerical stiffness. Under-relaxation has a much larger role in maintaining numerical stability than in reducing numerical stiffness (these issues are related, but not identical).

Adaptive Grid Techniques. The general approach to adaptive grid techniques is to resolve high gradient areas by being able to dynamically locate grids where they are most needed. There are two general ways to do this. A finite number of grids can be redistributed, or additional grids can be added in the regions where they are needed. An adaptive grid technique was successfully implemented into MAXIGAS and evaluated (Hedman, et al., 1985). The approach of the algorithm chosen was to add grids to an initially coarse grid structure. This is similar to multigrid techniques discussed below. While this technique did reduce computational time by 15-20%, it did not nearly meet the stated goal of making the amount of work proportional to the physical changes. The region where these grids were added is quite obvious for our geometries (near inlets) and does not require an extensive (and somewhat expensive) algorithm to determine. Also, some of the parameters used by this algorithm are difficult to determine except through trial and error.

For these reasons, and others, it is thought that for our applications multigrid techniques would provide superior results.

Multi-Grid Techniques. The goal of multigrid techniques is to use different grids, with different resolutions, to solve the specified problem. Only enough computational time is spent on each grid to solve the errors of the solution whose components correspond to the scale of that grid. Because the large scale errors of Figure 68 are not functions of grid refinement, it is most economical to solve them on as coarse a grid as possible. Conversely, the small scale errors exhibited in Figure 69 need to be resolved on a finer grid. By interactively employing multiple levels of grid refinement, the conflict between the scales of error components is eliminated, and numerical diffusion is greatly reduced.

A further advantage of multigrid techniques is the convenience of further refinement in subdomains. This is an important issue for possible use in 3-dimensional models where there are conflicts in the sizes of the reactor geometries and burners. This is one area that multigrid techniques have a distinct advantage over adaptive grid techniques. The derivation and theory of multigrid algorithms is given by (Brandt, 1984).

One multigrid cycle is thus defined by the following steps: 1) Variable smoothing (calculation of newer approximations) is performed on the finest grid structure, for one or more iterations (usually just a few iterations at most). 2) Principal variables (u, v, w, p) and their corresponding residuals at every node are interpolated onto the next coarsest grid. 3) Variable smoothing is performed again for a few iterations, incorporating both the variables and their residuals into the equations being solved. 4) Steps 2 and 3 are repeated recursively until the coarsest grid is reached. 5) Variable smoothing is continued on the coarsest grid until some convergence criteria is met. 6) Variable corrections are calculated and then interpolated onto the next finer grid. Previous values for these variables (corrections) on this grid are saved, so they can be corrected. 7) Variable smoothing is performed again for a few iterations. 8) Steps 5 and 6 are repeated until the finest grid level is reached.

The resolution of grid level i should be twice that of grid level $i-1$. Furthermore, the grids on any one level should be equidistant from each other. The multigrid cycles are repeated until some convergence criteria is met for the finest grid. Because of its mathematical foundation, multigriding is considered to be a potentially very attractive approach for PCGC-2 (and MAXIGAS). Chan and Saied, (1985) state that multigrid methods are computationally very competitive against other, more direct solution methods, for example pre-conditioned conjugant gradient methods. Following the approach advocated by Brandt, a detailed plan of development was established that would rigorously test each part of the multigrid process for maximum efficiency. The first major task accomplished was to convert the variable arrays in maxigas into one-dimensional arrays. Multi-dimensional arrays in multigrid processes are extremely wasteful of memory. The second task accomplished was to test and write the proper interpolation routines for our problem. The last task accomplished for this study was to code a two-level multigrid algorithm and begin debug efforts. For further evaluation of multigrid methods in PCGC-2 and MAXIGAS, see Christensen (1987).

Momentum-Continuity Coupling. A key part of any fluid-dynamics model is the coupling between momentum and continuity equations. It is most convenient to solve the momentum equations for their respective velocities. Because pressure is contained only in the momentum equations, some mathematical manipulation of the equations involved must be done in order to express pressure in the continuity equation. Because of this anomaly, one iterative step in the solution procedure usually has the following sequence: 1) The velocity fields are calculated from momentum equations based on some guessed pressure field. 2) The continuity equation is then satisfied, providing a new pressure field and corrections to the velocity fields. The SIMPLE/SIMPLER schemes currently used in PCGC-2 use this approach.

Distributed relaxation is a momentum continuity coupling method (Brandt, 1984) that takes advantage of staggered grids, and is in many ways similar to the SIMPLE/SIMPLER techniques currently used PCGC-2 and MAXIGAS. It will be shown later that SIMPLE/SIMPLER is a subset of distributive relaxation. In distributed relaxation, each of the momentum equations is solved sequentially for its respective velocity component, forcing the residual of each equation to go to zero. Then the continuity equation is solved, also forcing its residual to go to zero, but with the further restrictions that the residuals for the momentum equations remain constant. This step then provides corrections for the pressure and velocity fields.

In the SIMPLE/SIMPLER algorithms, this objective is almost followed, except that the residuals for the velocity equations are allowed to vary for all of the corrections. This is due to the fact that several terms in the velocity correction equations are ignored in SIMPLE/SIMPLER (see user's manual, Volume 2 of this report). If these terms were left in the equations, then SIMPLE/SIMPLER would, in result, be similar to distributed relaxation. However, these terms add considerable complexity to the SIMPLE/SIMPLER calculations. Because the approach to the continuity equation is different in distributed relaxation, these terms are not ignored, and it is thought to be a more efficient coupling technique.

Following the derivation by Brandt (1984) the velocity and pressure correction equations, for our coordinate system and equations, are

$$u_{i,j} = \tilde{u}_{i,j} - \frac{AUE_{i,j}}{AUP_{i,j}} \frac{1}{C_E} R_c \quad (27a)$$

$$\text{where } R_c = (-C_E \tilde{u}_{i-1,j} + C_W \tilde{u}_{i,j+1} - C_N \tilde{v}_{i,j+1} + C_S \tilde{v}_{i,j})$$

$$u_{i+1,j} = \tilde{u}_{i+1,j} + \frac{AUW_{i-1,j}}{AUP_{i+1,j}} \frac{1}{C_W} R_c \quad (27b)$$

$$v_{i,j} = \tilde{v}_{i,j} - \frac{AVN_{i,j}}{AVP_{i,j}} \frac{1}{C_N} R_c \quad (27c)$$

$$v_{i,j+1} = \tilde{v}_{i,j+1} + \frac{AVS_{i,j+1}}{AVP_{i,j+1}} \frac{1}{C_S} R_C \quad (27d)$$

$$(P_{i-1,j} - P_{i,j}) = (\tilde{P}_{i-1,j} - \tilde{P}_{i,j}) - \frac{AUE_{i,j} R_C}{D_u} \left(\frac{AUW_{i+1,j}}{AUP_{i+1,j}} \frac{1}{C_W} + \frac{1}{C_E} \right) \quad (28a)$$

$$(P_{i,j} - P_{i+1,j}) = (\tilde{P}_{i,j} - \tilde{P}_{i+1,j}) - \frac{AUW_{i+1,j} R_C}{D_u} \left(\frac{AUE_{i,j}}{AUP_{i,j}} \frac{1}{C_E} + \frac{1}{C_W} \right) \quad (28b)$$

$$(P_{i,j-1} - P_{i,j}) = (\tilde{P}_{i,j-1} - \tilde{P}_{i,j}) - \frac{AVN_{i,j+1} R_C}{D_v} \left(\frac{AVS_{i,j+1}}{AVP_{i,j+1}} \frac{1}{C_S} + \frac{1}{C_N} \right) \quad (28c)$$

$$(P_{i,j} - P_{i,j+1}) = (\tilde{P}_{i,j} - \tilde{P}_{i,j+1}) + \frac{AVS_{i,j+1} R_C}{D_v} \left(\frac{AVN_{i,j}}{AVP_{i,j}} \frac{1}{C_N} + \frac{1}{C_S} \right) \quad (28d)$$

where

$$R_C = C_W \tilde{U}_{i,j} - C_E \tilde{U}_{i-1,j} + C_X \tilde{V}_{i,j} - C_N \tilde{V}_{i,j+1}$$

$$C_W = C_E = \rho/2 (\Gamma_{i+1} + \Gamma_j) \Delta r$$

$$C_N = \rho \Gamma_{j+1} \Delta x$$

$$C_S = \rho \Gamma_j \Delta x$$

These corrections are made for every P-cell in the computational domain.

This algorithm has been coded and implemented into MAXIGAS, in conjunction with the multigrid algorithm, and debug efforts have begun.

Conclusions

During this study, a much more fundamental mathematical approach has been taken towards numerical efficiency. Considerable effort has been made in trying to better understand the numerical phenomena observed in PCGC-2 and MAXIGAS. Major mathematical improvements have been identified and evaluated for their impact on the codes.

Most of the previously discussed techniques have not been applied to a complex model such as PCGC-2. These techniques, if implemented in PCGC-2, may or may not provide the same dramatic improvements they do in simpler codes. However, used in a cumulative effort (new continuity-momentum coupling, with varying under-relaxation factors, and 3-4 level multigrid algorithm), these techniques should very significantly reduce the CPU requirements of PCGC-2, perhaps to 1/4-1/3 of the present requirements. The majority of this improvement will most likely come from multigriding.

Subtask 2.3 - Model Evaluation

Introduction

Data Book Comparisons. The objective of this subtask was to evaluate PCGC-2 on a general level to identify trends and patterns emerging through comparison of data and predictions. Additional funding from the Consortium contract (Contract No. DE-F822-85PC80752) allowed further research of the non-reacting gaseous and particle-laden flows as well as the gaseous and coal gasification/combustion. Trends found in these analyses were considered during performance evaluation of PCGC-2.

This subtask is aimed at evaluating submodel and overall model performance by comparing predictions to in-situ flow chamber, furnace or gasifier measurements. Specific tasks identified within this subtask were: 1) to converge the remaining sixteen cases in the Data Book (Smoot and Christensen, 1985) with PCGC-2, 2) to compare the resulting predictions with the experimental data, 3) and to analyze the other Data Book cases to identify possible limitations in the model and to identify errors in the Data Book or in the original experimental technique, and 4) to apply the model to measurements made in this study.

In 1985, BYU compiled a set of gasification-related data from various investigators. This collection (referred to as the Data Book) provides a single reference containing detailed experimental data for use in model evaluation. The five categories contained within the Data Book are: 1) gaseous cold flow, 2) particle-laden cold flow, 3) gaseous combustion, 4) coal combustion, and 5) coal gasification. Many of the cases contained in the Data Book have been modeled with PCGC-2 and analyzed by past investigators (Hill, 1980; Fletcher, 1983; Sloan, 1985). Work for this project included computations for sixteen of the 35 cases that had not been analyzed previously with PCGC-2. The Data Book was also reviewed for errors and corrections were made.

A summary table of the sixteen cases recently modeled with PCGC-2 appears in Table 19. This table includes a classification of cases, a reference to the investigator who originally collected the data, and a short description of the chemical system. The specific results of each simulation and general observations from each data type are summarized. Each of the data classifications will be addressed, beginning with gaseous cold flow and ending with coal gasification. This subtask was performed principally by Rasband (1987) and the majority of this subtask report has been extracted from this thesis, where further details are shown.

Gaseous Cold Flow. The modeling of gaseous cold flows is an important tool in evaluating the turbulence submodel for gasification and combustion applications. Two non-reacting cases (Takagi, 1980; and Webb, 1982) were modeled with PCGC-2 for this study.

Takagi et. al. (1980) recorded instantaneous measurements of mean axial velocities, temperature, and species concentrations in turbulent ($Re = 4200$) hydrogen-air systems. The species compositions were detected by a gas chromatograph and the velocities and turbulence characteristics were obtained with LDV. This case is unusual because it presents a large density gradient between the primary and secondary stream without a temperature gradient. This

TABLE 19
SUMMARY OF DATA BOOK CASES MODELED DURING THIS STUDY

<u>No.</u>	<u>Category</u>	<u>Investigator</u>	<u>System</u>
1	Gaseous Cold Flow	Takagi et. al., 1980 (Osaka Univ.)	Hydrogen/Air
2	Gaseous Cold Flow	Webb, 1982 (BYU)	Air/Air
3	Particle-Laden Cold Flow	Sharp, 1981 (BYU)	Silicon/Air
4	Particle-Laden Cold Flow	Modaress et. al., 1982 (U.C. Irvine)	Silicon/Air
5	Particle-Laden Cold Flow	Modaress et. al., 1982 (U.C. Irvine)	Silicon/Air
6	Particle-Laden Cold Flow	Leavitt, 1980 (BYU)	Coal/Air
7	Particle-Laden Cold Flow	Leavitt, 1980 (BYU)	Coal/Air
8	Particle-Laden Cold Flow	Leavitt, 1980 (BYU)	Coal/Air
9	Gaseous Combustion	Michelfelder & Lowes, 1974 (IFRF)	Propane/Air
10	Gaseous Combustion	Michelfelder & Lowes, 1974 (IFRF)	Methane/Air
11	Gaseous Combustion	Takagi et. al., 1980 (Osaka Univ.)	Nitrogen/ Hydrogen/Air
12	Gaseous Combustion	Hassan et. al., 1983 (Imperial College)	Natural Gas/Air
13	Gaseous Combustion	Michelfelder & Lowes, 1974 (IFRF)	Methane/Air
14	Gaseous Combustion	Gouldin et. al., 1983 (Cornell)	Natural Gas/Air*
15	Coal Combustion	Hein & Leuckel, 1970 (IFRF)	Anthracite/Air
16	Coal Combustion	Michel and Payne, 1980 (IFRF)	Bituminous/Air

*Unsuccessful attempts were made to converge this case. However, converged solutions for these cases have been completed at this laboratory previously (Sloan, et al., 1986).

case was modeled with various estimates of the inlet turbulence intensity and turbulent Schmidt Number. Initially, the centerline axial velocity predictions decayed prematurely, while the radial profiles show an overprediction of the velocity in the outer regions of the reactor. By reducing the inlet turbulence intensity from a recommended value to its measured value, a vast improvement resulted. A local maximum found in the predictions but not in the data was removed and the RMS axial velocity predictions qualitatively match the data. These results are shown in Figure 70 which compares model predictions using two values of the inlet turbulence intensity and Takagi's data.

Webb (1982) performed laser doppler anemometer measurements in a coaxial air jet with sudden expansion and a moveable block swirler in the secondary stream. Due to the inadequacy of the LDA seed used by Webb, an azimuthal velocity map was not recorded. Comparisons were made of mean and rms axial velocity with model predictions. Integrated axial velocity distributions at downstream locations were as much as 30% in error relative to the metered flow rates. Comparisons show that the experimental data are skewed toward the chamber wall with less of a velocity deficit along the centerline in comparison to the predictions. Measured velocities appeared to decay faster than the predictions.

From these data sets and previous evaluations of PCGC-2's capability to model non-reacting flow, some observations were made. First, the code has a tendency to overpredict mixing in non-swirling flows and underpredict mixing in swirling flows. Second, the accuracy of inlet turbulence intensity is important. Third, rms velocities do not agree well in complex turbulent flows, such as recirculation zones, flow separation, or high tangential velocities.

Particle-Laden Cold Flow. Six non-reacting, two phase flow data sets were modeled for this study. The detailed effects of particles on the gaseous flow field in turbulent combustion are not completely understood and the study of turbulent dispersion of the particle phase is important in better understanding the coal gasification and combustion process.

Sharp (1981) used an "isokinetic" collection probe to measure argon concentration and particle flux in turbulent confined jets seeded with silicon beads. The PCGC-2 centerline axial velocity profiles showed a more rapid mixing in the predictions than is evidenced in the data. The particle flux comparisons are accurately described by the comprehensive model.

Modarress and Wuerer (1982) made LDA measurements of flow properties in a confined, two-phase turbulent jet system. The silicon particle size was varied from 200 microns for the first data set to 50 microns for the second data set. The smaller particle case illustrated that smaller particles interact more with turbulent fluctuations and their behavior more closely parallels the gaseous axial velocity decay than the larger particles. The centerline mean velocity profile at the confluence plane shows a very slight overprediction (1.5%), but it quickly degenerates to an overprediction of 20% farther down the reactor. PCGC-2 predicts a radial profile flatter in shape than the data but with the same areas of maximum and minimum flow.

Figure 70. Effect of inlet turbulence intensity on RMS axial velocity predictions for non-reacting turbulent hydrogen-air (data from Tagaki, et al, 1980).

Figure 71. Prediction of centerline Argon concentration for an argon-air-coal laden jet with swirling flow (data from Leavitt, 1980).

Leavitt (1980) recorded argon concentrations and particle flux in turbulent confined jets. Data were collected at three conditions; low swirl number, low swirl number with a quarl, and high swirl number. After correcting reported inlet conditions according to a mass balance of the exit conditions, good agreement was obtained between the model predictions and data. Figure 71 shows the difference in agreement when the inlet conditions are corrected according to the outlet conditions. Discrepancies did not exceed ten percent anywhere along the reactor, and the degree of mixing is accurately characterized. The second data set revealed increased mixing due to the addition of a quarl. This trend was correctly predicted by PCGC-2, but this case contained predicted argon concentrations that were consistently higher than the measured values unless the inlet conditions are again adjusted. The third case showed the same trends evident in the first two cases.

Generally, it was observed that non-swirling flows show faster velocity decay, or more rapid mixing, in the predictions than the data, while the swirling cases show the opposite effect. Mixing qualities were significantly affected by adjusting inlet velocity profiles. For the Leavitt cases, it appeared that when the turbulence of the particle-laden system increases, the departure of the argon predictions from the data is more pronounced.

Gaseous Combustion. Three of the six gaseous combustion data sets modeled by the code for this subtask were collected by Michelfelder and Lowes (1974). These three cases, propane with and without swirl and methane without swirl, were specifically intended to aid in the development of combustor models. Although the combustor used in this study was rectangular, radial profiles of species composition and temperature show a very near-perfect symmetry. Centerline profiles of temperature, O_2 , CO, and CO_2 were compared with data. PCGC-2 temperature predictions show the same basic pattern as the data with a few minor exceptions, as seen in Figure 72. Centerline predictions for CO_2 were reasonable, but the CO and O_2 comparison yielded less reliable results. However, the radial profiles of O_2 and CO are reassuring. The poor centerline predictions could be the result of incorrect data, premature micromixing, or the inability of the code to correctly model the heat loss. The methane case predictions were also affected by heat losses in the combustor. The third case involved block type swirl generator in the secondary stream. Centerline temperature profiles are again reasonable although predictions tended to rise quicker and taper sooner than was observed. The CO profiles show good qualitative agreement, but the CO_2 and O_2 predictions deviate significantly from the data.

Other gaseous combustion data sets modeled were the Takagi, et al. (1981) case, the Hassan, Lockwood, and Moneib (1983) case, and the Gouldin (1983) cases. Centerline axial predictions of the Takagi case compared favorably, although there was a slight tendency to underpredict in the front of the reactor. The temperature rise and flame location also were prematurely predicted. This case illustrated that hydrogen diffusion flames can be adequately modeled using the assumption of mixing-limited reactions. The reactor used by Hassan et. al. (1983) was difficult to model due to its unusual cooling configuration. Because the flame front was not adequately predicted, no further analysis was conducted. The two cases by Gouldin, Depsky, and Lee (1983) were not successfully converged with PCGC-2, in this study, but were previously simulated (Sloan, et al., 1986).

Figure 72. Temperature predictions and data for gaseous combustion of propane-air (data from Michelfelder and Lowes, 1974).

Figure 73. Centerline temperature profile for coal combustion in air (data from Michel and Payne, 1980).

Coal Combustion. The foregoing analyses have been foundational for the prediction of coal combustion and gasification data. Two different coal combustion cases were converged for this subtask. The first case, Hein and Leuckel (1970) has been successfully run and a complete analysis of the results is being conducted in a separate study (Rasband, 1987).

Michel and Payne (1980) characterized a coal flame in a 1.9 m by 1.9 m rectangular reactor. Temperature predictions indicate a tendency to rise more steeply than the data in the forward regions of the reactor and the flame front is prematurely predicted as illustrated in Figure 73. PCGC-2 was able to accurately model the recirculation zones for this case and the radial temperature profiles are fairly well predicted. Centerline comparison of species concentrations reflect the difference in the flame front location. Comparison of O_2 and CO_2 centerline profiles yield remarkable agreement but the centerline CO profile agreement is marginal. This case shows that the discrepancies between the code and data can not be attributed mainly to the devolatilization parameters, but some of the discrepancy can be attributed to the turbulence model.

Coal Gasification. Coal gasification processes are similar to those of fuel-rich coal combustion. For this reason, methods of modeling coal gasification processes are consistent with those for coal combustion. All of the previous comparisons of simpler flows were essential to evaluation of different components of the gasification process. All gasification cases in the original Data Book have been previously successfully modeled with PCGC-2 (Smoot and Christensen, 1985).

Gasification Applications

Several recently completed gasification tests as part of this contract were modeled with PCGC-2. This work is reported in detail in Section II of this report. A brief summary of PCGC-2 gasification evaluation runs are given in Table 20.

Generally, good qualitative agreement is exhibited in profile comparisons of model predictions and experimental data for CO, CO_2 , and H_2 concentrations. In the higher-volatile coals, discrepancies exist near the reactor inlet. Some noted trends in gasification are: 1) centerline CO_2 show a characteristic peak in the near-inlet region, 2) CO radial profiles show a marked overprediction of CO in the aft section of the gasifier, 3) trends were predicted correctly for the effect of steam/coal ratio on exit CO/ CO_2 ratio, and 4) centerline CO predictions are skewed to the left for gaseous diffusion and coal combustion flames.

TABLE 20

SUMMARY OF GASIFICATION PREDICTIONS FOR COMPARISON WITH
MEASUREMENTS (See Section II)

<u>Type of Prediction</u>	<u>No. of Solutions</u>	<u>Variables</u>
Premixed flame Parallel Injection	13	O ₂ Partitioning Injector A
Diffusion flame Parallel Injection	13	O ₂ Partitioning Injector B
Diffusion flame Swirled Primary	13	O ₂ Partitioning Injector C
Diffusion flame Impinging Secondary	17	O ₂ Partitioning Injector D
NO _x predictions for each injector type	4	Effect of injector on NO _x formation
NO _x predictions for test matrix	9	Effect of feedrate and pressure on NO _x formation
	—	
Total	69	

IV. TASK 3: APPLICATION TO INDUSTRIAL AND METC NEEDS

Subtask 3.1 - Technical Papers, Seminars, and Reports

Contract Reports

Monthly technical and financial reports were regularly submitted on the contract. In addition to this Final Report, the following Quarterly Technical Progress Reports were submitted:

Lindsay, J.D., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," First Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (June 30, 1985).

Lindsay, J.D., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Second Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (September 30, 1985).

Lindsay, J.D., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Third Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (December 31, 1985).

Hedman, P.O., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Fourth Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (March 31, 1986).

Hedman, P.O., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Fifth Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (June 30, 1986).

Hedman, P.O., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Sixth Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (September 30, 1986).

Hedman, P.O., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Seventh Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (December 31, 1986).

Hedman, P.O., and Smoot, L.D., "Entrained Flow Gasification at Elevated Pressure," Eighth Quarterly Progress Report, USDOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (March 31, 1987).

In addition to these reports, two additional volumes are contained in this final report.

Smith, P.J., Smoot, L.D. and Brewster, B.S., User's Manual for PCGC-2. Volume 2 (1987) Final Report, U.S. DOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (1987).

Rasband, M., Christensen K.R., and L.D. Smoot, "Prediction and Measurement of Entrained Flow Coal Gasification Processes; Volume 3 - Data Book," Final Report, U.S. DOE Contract No. DE-AC21-85MC22059, Combustion Laboratory, Brigham Young University, Provo, Utah (1987).

Theses and Dissertations

The following Master's Theses and Ph.D. Dissertations relating to this study were completed as part of the contractual effort:

Brown, B.W., "Effect of Coal Type on Entrained Gasification," Ph.D. Dissertation, Chemical Engineering Department, Brigham Young University, Provo, Utah (1985).

Nichols, K.M., "The Effects of Elevated Pressure on Nitrogen and Sulfur Pollutant Formation During Coal Gasification," M.S. Thesis, Chemical Engineering Department, Brigham Young University, Provo, Utah (1985).

Lindsay, J.D., "LDA Measurements in a Simulated Gasifier with Swirl," Ph.D. Dissertation, Chemical Engineering Department, Brigham Young University, Provo, Utah (1986).

Baxter, L.L., "Particle Phase Behaviour in Combustion Environments", Ph.D. Dissertation, Chemical Engineering Department, Brigham Young University, Provo, Utah (1987).

Christensen, K.R., "Improving the Numerical Efficiency of a Two-Dimensional Coal Combustion Model," M.S. Thesis, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Rasband, M.W., "A Combined Analysis of the Data Book and PCGC-2," M.S. Thesis, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Sowa, W.A., "The Effect of Injector Design on the Performance of the BYU Gasifier," Ph.D. Dissertation, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Nichols, K.M., "Nitrogen Chemistry in a High-Pressure Entrained-Coal Gasifier," Ph.D. Dissertation, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Cope, R., "The Effects of Coal Rank on Pressurized Entrained Coal Gasification," M.S. Thesis, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Smith, M.W., "The Effects of Coal Rank on the Formation of Nitrogen and Sulfur Pollutants During Coal Gasification," M.S. Thesis, Chemical Engineering Department, Brigham Young University, Provo, Utah (in progress 1987).

Copies of these documents are available to DOE upon request at no cost and to others for copy, handling, and mailing costs.

Technical Publications

The following reviewed publications relating to this research study were published during the contract period:

Smoot, L.D., and Smith, P.J., Coal Combustion and Gasification, Plenum, Press, New York, NY, 443 pgs. (1985).

Soelberg, N.R., Smoot, L.D., and Hedman, P.O., "Entrained Flow Gasification of Coal 1. Evaluation of Mixing and Reaction Processes from Local Measurements," Fuel, 64, 776-781 (1985).

Highsmith, J.R., Soelberg, N.R., Hedman, P.O., Smoot, L.D. and Blackham, A.U., "Entrained Flow Gasification of Coal 2. Fate of Nitrogen and Sulfur Pollutants as Assessed from Local Measurements," Fuel, 64, 782-788 (1985).

Azuhata, S., Hedman, P.O. and Smoot, L.D., "Carbon Conversion in an Atmospheric-Pressure Entrained Gasifier," Fuel, 65, 212 (1986).

Brown, B.W., Smoot, L.D., and Hedman, P.O., "Effect of Coal Type on Entrained Gasification," Fuel, 65, 673-678 (1986).

Azuhata, S., Hedman, P.O., Smoot, L.D. and Sowa, W.A., "Effects of Flame Type and Pressure on Entrained Coal Gasification," Fuel, 65, 1511 (1986).

Sloan, D.G, Smith, P.J. and Smoot, L.D., "Modeling of Swirl in Turbulent Flow Systems," Progress in Energy and Combustion Science, 12, 163-250 (1986).

Nichols, K.M., Hedman, P.O. and Smoot, L.D., "Release and Reactions of Fuel-Nitrogen in a High-Pressure Entrained-Coal Gasifier," Fuel, 66, 1257-1263 (1987).

Smoot, L.D. and Brown, B.W., "Controlling Mechanisms in Gasification of Pulverized Coal," Fuel, 66, 1249-1256 (1987).

Other papers based on the work of Sowa (1987), Nichols (1987), Cope (1987), Smith (1987), Baxter (1987), Christensen (1987), and Rasband (1987) were in preparation for journal publications at the time this final report was published.

Technical Presentations

The following presentations were made at technical conferences during the contract period:

Smith, P.J. and Baxter, L.L., "A Study of Turbulent Particle Dispersion in Pulverized Coal Combustion and Gasification," 1986 Spring Joint Meeting of the Western States and Canadian Sections of the Combustion Institute, Banff, Alberta, Canada, (April 28-30, 1986).

Lindsay, J. D., Hedman, P. O. and Smith, P. J., "LDA Measurements in a Simulated Gasifier with Swirl," Third International Symposium on Applications of Laser Anemometry to Fluid Mechanics, Lisbon, Portugal (July 7-9, 1986).

Nichols, K.M., Hedman, P.O. and Smoot, L.D., "Release and REactionsof Fuel-Nitrogen in a High-Pressure Entrained-Coal Gasifier," Western States Section, Combustion Institute (October 27-28, 1986).

Sowa, W.A., Hedman, P.O., Smoot, L.D. and Blackham, A.U., "The Behavior of Chlorine in Illinois Coals during Combustion and Its Effects on Ash Deposits," Western States Section, Combustion Institute (October 27-28-1986).

Smith, P.J., Sowa, W.A. and Hedman, P.O., "Furnace Design and Comprehensive Coal Combustion Models," Symposium on Furnace Modeling, ASME Winter Annual Meeting, Anaheim, California (December, 1986).

Nichols, K.M., Hedman, P.O. and Smoot, L.D., "Sulfur Species Formation in a High-Pressure Entrained-Coal Gasifier," Western States Section, Combustion Institute (April 6-7, 1987).

Subtask 3.2 - Data Book

The initial version of the Data Book (Smoot and Christensen, 1985) was published in 1985. It was designed to aid in the development of computer models for coal combustion and gasification. The main task of this project was to identify the errors due to typographical problems within the original document as well as those due to transposing. These errors were located, noted and subsequently corrected. A revised edition of the Data Book is included as Volume 3 of this report. A brief description of the book follows.

The Data Book (Smoot and Christensen, 1985) was prepared for the U.S. Department of Energy under Contract No. DE-AC21-81MC16518. It was not intended to be a consummate review of combustion and gasification related data. Rather, it was established to provide a convenient and reliable source of data for modeling purposes. To allow independent analysis of different model components, the Data Book was divided into five, increasingly complex categories: 1) gaseous cold flow, 2) particle-laden cold flow, 3) gaseous diffusion flames, 4) coal combustion flames, and 5) coal gasification. Each category was further subdivided into swirling and non-swirling cases (with the exception of the gasification section which only contained non-swirling flows).

Aside from relevancy to gasification and combustion, several criteria were established for data selection. The first set of criteria was devised to insure 1) data consistency, 2) axial symmetry in the geometry, 3) steady-state conditions of the system, and 4) that the detail in the data profiles was adequate. In a few cases (e.g. Michelfelder, et al., 1974), data were recorded for combustion in a rectangular reactor, but an examination of the data revealed near axisymmetric throughout the chamber. Therefore, these data were incorporated in the revised Data Book and considered "axisymmetric". Although not as stringently required as the previous standards, the following

characteristics were desired of each data case selected: 1) well defined initial boundary conditions, 2) diverse and detailed variables, 3) current and reliable tools and techniques for data collection, 4) data available in tabular form, and 5) representative sampling over the length of the reactor. Some allowances were made for this last list of criteria, but with no significant detriment to the integrity of the data. System-related errors, or "inbreeding", was avoided by accumulating sets from various test facilities, and systematic error was minimized by selecting data gathered under different operating conditions. The revised set of data have been prepared, corrected, and are included as Volume 3 of this report. Table 21 summarizes general information pertaining to each set of data.

Subtask 3.3 - Code Placement

Over the past several years, the BYU Combustion Laboratory has placed copies of 1-DICOG (1-Dimensional Combustion or Gasification) and PCGC-2 (Pulverized Coal Gasification and Combustion-2 Dimensional) at several organizations in the U.S. and in foreign countries. A summary of these organizations is shown in Table 22. As shown, 60 organizations currently have BYU combustion codes, 39 have PCGC-2, and 21 have 1-DICOG. Seven organizations have acquired PCGC-2 during the period of this contract, one has acquired 1-DICOG, and several others (not shown) have inquired and are in the process of obtaining one or the other of the codes.

The Combustion Laboratory hired a full-time research associate, Dr. B. Scott Brewster, during the last year to help manage code distribution. During the last year, the user manual for PCGC-2 was revised, a new version of PCGC-2 was released for distribution, and plans were initiated for forming a user's group. A formal licensing agreement and policy for code distribution were also developed.

During the last three months of the study, approximately 60 survey forms were mailed to current code users and industrial supporters of the laboratory to determine the level of interest in forming a users group, what services that should be provided, and what would be a reasonable cost. Out of 27 responses, 14 have indicated medium or high interest in forming a users group, and the organization of a PCGC-2 Users Group is proceeding.

TABLE 21

DATA BOOK: GENERAL INFORMATION

<u>Category</u>	<u>Investigator</u>	<u>Chem. System</u>	<u>Recorded Measurements</u>	<u>Swirl No.</u>	<u>Measurement Techniques</u>
Gaseous Cold Flow	Owen (Arco, Inc.)	Air/Air	U, V	----	LDV
Gaseous, Cold Flow	Takagi, et al. (Osaka Univ.)	H ₂ /Air	H ₂ , N ₂ , O ₂ , U, <V>, <W>, <U>	----	LDV, stainless steel water-cooled probe
Gaseous, Cold Flow	Webb (BYU)	Air/Air	U, <U>	----	LDV (without frequency shifting)
Gaseous, Cold Flow	Samuelson, et al. (U.C. Irvine)	CO ₂ /Air	U, <U>, W <W>	0.3, 0.0 0.8, 0.0	LDV
Gaseous, Cold Flow	Webb (BYU)	Air/Air	U, <U>, V, <V>	0.0, 0.49	LDV (without frequency shifting)
Gaseous, Cold Flow	Gouldin, et al. (Cournell Univ.)	Air, Air	U, <U>, V, <V>	0.5, 0.56 0.5, -0.56	LDV
Part.-Laden Cold Flow	Leavitt (BYU)	Coal/Air	Ar, PFLUX	----	Collection Probe
Part.-Laden Cold Flow	Sharp	Silicon/Air	Ar, PFLUX	----	Collection Probe
Part.-Laden, Cold Flow	Modarress, et al. (U.C. Irvine)	Silicon/Air	U, <U>, <V>, PURMS, PUVÉ	----	LDV
Part.-Laden, Cold Flow	Modarress, et al.	Silicon/Air	U, <U>, <V>, PURMS, PUVÉ	----	LDV
Part.-Laden, Cold Flow	Leavitt (BYU)	Coal/Air	Ar, PFLUX	0.0, 0.40	Collection Probe
Part.-Laden, Cold Flow	Leavitt (BYU)	Coal/Air	Ar, PFLUX	0.0, 0.40	Collection Probe

TABLE 21 (Continued)

Category	Investigator	Chem. System	Recorded Measurements	Swirl No.	Measurement Techniques
Gaseous Combustion	Michelfelder (IFRF)	Propane/Air	O ₂ , N ₂ , CO ₂ , H ₂ , Temp.	----	Water-cooled probe, suction pyrometer
Gaseous Combustion	Michelfelder (IFRF)	Methane/Air	O ₂ , N ₂ , CO ₂ , H ₂ , Temp.	----	Water-cooled probe, suction pyrometer
Gaseous Combustion	Takagi, et al. (Osaka Univ.)	N ₂ , H ₂ /Air	O ₂ , N ₂ , H ₂ O, H ₂ , U, <U> V, <V>	----	LDV, suction pyrometer
Gaseous Combustion	Hassan (Imperial College)	Nat. Gas/Air	O ₂ , CO, CO ₂ , Temp.	----	Water-cooled probe, gas-temp. thermocouple
Coal Combustion	Hein (IFRF)	Anthra./Air	O ₂ , N ₂ , CO ₂ , Temp.	0.0, 1.4	Water-cooled probe, suction pyrometer
Coal Combustion	Harding (BYU)	Anthra./Air	O ₂ , N ₂ , CO ₂ , H ₂ , Ar, CO, H ₂ O, CH ₄ , HCN, NH ₃	0.0, 2.2	Water-quenched iso-kinetic probe
Coal Combustion	Asay (BYU)	Anthra./Air	O ₂ , CO, CO ₂ , H ₂ , Ar, N ₂ , NO, H ₂ O, NH ₃ , HCN, CH ₄ , C, H, N, O-S, Ash	0.0, 2.0	Water-quenched iso-kinetic probe
Coal Gasification	Soelberg (BYU)	Bitum./Air	O ₂ , CO, CO ₂ , H ₂ , Ar, N ₂ , NO, NH ₃ , HCN, Ash, H, CS ₂ , SO ₂ , COS, H ₂ S, C	----	Water-quenched iso-kinetic probe
Coal Gasification	Brown (BYU)	Subbit./Air	Ar, He, CO ₂ , CO, CH ₄ , S, H ₂ , O ₂ , C, H, O, Ash, N	----	Water-quenched iso-kinetic probe
Coal Gasification	Brown (BYU)	Lignite/Air	Ar, He, CO ₂ , CO, CH ₄ , S, H ₂ , O ₂ , C, H, O, Ash, N	----	Water-quenched iso-kinetic probe
Coal Gasification	Brown (BYU)	Bitum./Air	Ar, He, CO ₂ , CO, CH ₄ , S, H ₂ , O ₂ , C, H, O, Ash, N	----	Water-quenched iso-kinetic probe
Gaseous Combustion	Michelfelder (IFRF)	Methane/Air	O ₂ , N ₂ , CO ₂ , H ₂ , Temp.	0.0, 0.80	Water-cooled sampling probe, suction pyrometer

TABLE 21 (Continued)

Category	Investigator	Chem. System	Recorded Measurements	Swirl No.	Measurement Techniques
Gaseous Combustion	Samuelson (U.C. Irvine)	Propane/Air	U, W, <U>, <W>, U-W	0.0, 0.80	LDV
Gaseous Combustion	Gouldin, et al. (Cornell)	Nat. Gas/Air	U, <U>, V, <V>	0.5, 0.56 0.5,-0.56	LDV
Coal Combustion	Beér (MIT)	Anthra./Air	O ₂ , CO ₂ , Temp.	----	Suction pyrometer, T-suction pyrometer
Coal Combustion	Hein (IFRF)	Anthra./Air	O ₂ , N ₂ , CO ₂ , Temp.	----	Water-cooled sample probe
Coal Combustion	Thurgood (BYU)	Bitum./Air	O ₂ , CO, CO ₂ , H ₂ , NO C, Ar, H, S, O	----	Water-quenched, iso-kinetic probe
Coal Combustion	Michel & Payne (IFRF)	Bitum./Air	O ₂ , CO, CO ₂ , H ₂ , NO, N, Ash, Temp.	----	Water-cooled probe, suction pyrometer
Coal Combustion	Rees (BYU)	Bitum./Air	O ₂ , CO, CO ₂ , H ₂		Water-cooled probe, suction pyrometer
Coal Combustion	Hein (IFRF)	Anthra./Air	O ₂ , N ₂ , CO ₂ , Temp.	0.0, 1.0	Water-cooled probe, suction pyrometer

TABLE 22
ORGANIZATIONS WITH BYU COMBUSTION CODES

<u>Company</u>	<u>City</u>	<u>State</u>	<u>Country</u>	<u>PCGC-2</u>	<u>1-DICOG</u>
Advanced Fuel Research	East Hartford	CT	USA	x	x
Allison Gas Turbine	Indianapolis	IN	USA	x	
Argonne National Laboratory	Argonne	IL	USA	x	
Babcock & Wilcox R&D Division	Alliance	OH	USA	x	
Battelle Memorial Institute	Columbus	OH	USA	x	x
Bertin and Cie	Versailles		France	x	x
Brigham Young University	Provo	UT	USA	x	x
British Gas			England	x	x
Coen Company	Burlingame	CA	USA	x	x
Consolidated Coal Company	Library	PA	USA	x	
DOE/METC	Morgantown	WV	USA	x	x
DOE/PETC	Pittsburgh	PA	USA	x	x
Dow Chemical U.S.A.	Plaquemine	LA	USA	x	
Electric Power Research Institute	Palo Alto	CA	USA	x	x
Energiteknik Utveckling AB	Stockholm		Sweden	x	
EVT	Stuttgart		Germany	x	
Exxon Research & Engr. Division	Linden	NJ	USA		x
Eyring Research Institute	Provo	UT	USA	x	
Foster Wheeler Development Corp.	Livingston	NJ	USA	x	x
General Electric Corp. Res. & Dev.	Schenectady	NY	USA	x	
Harwell			England	x	
Hercules Aerospace	Magna	UT	USA	x	
Hitachi America, Ltd.	New York	NY	USA	x	
IHI Heavy Industries Co., Ltd.	Tokyo		Japan	x	x
IRSID	Maizieres les Metz		France	x	
Kobe Steel	Tokyo		Japan	x	x
Laboratoires du Cherchar	Cherchar		France	x	
Los Alamos National Laboratory	Los Alamos	NM	USA	x	
Massachusetts Inst. of Technology	Cambridge	MA	USA	x	
Mt. Energy Resources	Butte	MT	USA	x	
National Aeronautics & Space Admin.	Cleveland	OH	USA		x
National Defense Research Inst.			Sweden	x	
Natural Resources Research Inst.	Duluth	MN	USA	x	
Nuclear Technical Services	Ann Arbor	MI	USA	x	x
Phillips Petroleum Co.	Bartlesville	OK	USA		x
Power Computing Co.	Dallas	TX	USA	x	
Rockwell International	Canoga Park	CA	USA		x
Sandia National Laboratories	Livermore	CA	USA	x	x
Southern Company Services	Birmingham	AL	USA	x	x
Standard Oil Co.	Cleveland	OH	USA		x
Tennessee Valley Authority	Chattanooga	TN	USA	x	
University of Alabama	Tuscaloosa	AL	USA	x	
University of Utah	Salt Lake City	UT	USA	x	
U.K. Atomic Energy Authority	Didcot	Oxon	England	x	
Wayne State University	Detroit	MI	USA		x
Count:	60			39	21

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APPENDICES

INTRODUCTION

Appendices A, B and C contain summaries of the parametric variation tests performed for Subtask 1.1a, the mapping tests performed for Subtask 1.1b, and the parametric variation tests and mapping tests for subtask 1.2, respectively.

The values presented in these tables are output of the data reduction code developed during this study (see Sowa 1987). Because the reported values are output from the code the following items should be noted:

The numbers of significant figures shown were chosen as a matter of formatting convenience and are not justified in some cases, e.g. four significant figures for carbon conversion.

Some test numbers are not reported, because an acceptable mass balance closure was not obtained in reducing the data obtained from that test.

Negative values were obtained in some instances for N_2 (normalized water-free gas analysis) and O_2 (char analysis) because these values are obtained by difference. Negative values of S (elemental closure) in some tests are attributed to difficulty in accurately measuring sulfur concentrations in the samples.

Table 23 provides a glossary of terms used in the first three appendices.

TABLE 23

GLOSSARY OF TERMS USED IN EXPLANATION OF DATA TABLE ENTRIES
FOR APPENDICES A, B AND C

<u>Entry</u>	<u>Comment</u>
Coal Type	<p>Applies only to tests in subtask 1.1 Possible coal types include: North Dakota lignite Wyoming subbituminous coal Illinois No. 6 bituminous coal</p> <p>All cases that do not list a coal type used Utah bituminous coal.</p>
Test Number (dimensionless)	<p>All tests conducted during contract period were numbered in chronological order without respect to specific subtask. Incomplete data sets and unrealistic data sets are not included in data tables.</p> <p>A test number with a * following refers to a sample where the O_2/coal ratio falls significantly outside of the range 0.7-1.0.</p>
Flowrates (kg/hr)	The coal flowrate is on a wet basis. H_2O represents the steam flow rate. The purge gas is N_2 for all samples except nos. 271-284 where the purge was Ar.
Gas Analyses (mole percent)	The tabulated measured species concentrations for Ar, CO, CO_2 , CH_4 , H_2 , O_2 , and N_2 were normalized to be on a water and pollutant free basis. Air contamination corrections were used to obtain N_2 , O_2 and Ar values in sample numbers 80-146, 170-198, 206-226, 253-260. All gas analyses corrections are discussed in the text.
Char Analyses (mass percent)	C, H, and N were measured on a LECO Elemental Analyzer, S was measured on a LECO Sulfur Analyzer, ash was measured in accordance with ASTM procedures for proximate ash determination, O was determined by difference. No attempt was made to modify the elemental composition measurements.
Code (dimensionless)	<p>Applies only to tests in subtask 1.2 Defines Injector type and Test Series</p> <p>A - Injector B, optimization B - Injector B, mapping (5.5 atm) C - Injector C, optimization D - Injector C, mapping (5.5 atm) E - Injector D, optimization F - Injector D, mapping (5.5 atm) G - Injector C, mapping (1.0 atm)</p>

TABLE 23 (Continued)

All cases that do not list a code used a premixed primary stream injector.

Probe Location (cm)	Axial distance from injector tip, radial distance from centerline.
Mass Ratios (kg/kg)	Input parameters O_2 /coal ratio, steam/coal ratio, total input moisture/coal ratio, and predicted water leaving the gasifier relative to the total input moisture (OII).
Pressure (atmosphere)	Reactor chamber pressure, measured at the reactor exhaust.
Mole % H_2O in gas (mole percent)	Calculated exhaust gas water mole fraction by local mass balance equations.
MW gas (kg/kg-mole)	Molecular weight of the exhaust gas (dry basis).
Conversion (mass percent)	Elemental and total conversion for coal. The elemental conversion is on a moisture, ash and other element free basis. The total conversion is on a moisture free basis.
Mixing Parameters (dimensionless)	<p>Computed values for progress variables n, γ and f determined from solutions of local mass balance equations. Definitions:</p> <p>n = original coal mass in local gas sample divided by total mass of local gas sample.</p> <p>γ = mass window purge gas in local gas sample divided by local mass of primary, secondary and window purge gas.</p> <p>f = mass primary gas in local gas sample divided by local mass of primary and secondary gas in sample.</p> <p>adj. n = original coal mass in local gas sample divided by local mass of original coal mass, primary and secondary gas in the local gas sample.</p>
Viscosity (micro-Poise)	Estimated gas viscosity at the exit plane determined using a modified Chapman-Enskog approximation suggested by Brokaw and uncorrected bare thermocouple temperature measurements at the exit plane.
Reynold's Number (dimensionless)	Estimated Reynold's number at the exit plane based on exhaust gas mass flow rate and estimated gas viscosity.

TABLE 23 (Continued)

Measured/Calculated (mole/mole)	Ratio of experimentally measured local elemental molar concentrations to the calculated local elemental molar concentrations based upon the local mass balance equation.
Mass(out)/Mass(in) (kg/kg)	Ratio of elemental and total mass flow rates out of the gasifier to the elemental and total input flow rates. A flat mass flux profile was assumed in computation.
Energy Balance (kW-hr/kW-hr)	Ratio of sensible and internal energy contained in output gas and char relative to the internal energy of the input coal. The sensible energies of the input coal and gases are not shown. The "energy lost" term represents energy that was not attributable to the output gases and char and was found by difference. The sensible heat out of the system was based upon the outlet temperature measured by the bare uncorrected thermocouple at the exit of the gasifier. Corrected temperatures would raise the sensible heat terms and decrease the "energy lost" term.
Outlet Temperature (K)	Uncorrected bare thermocouple gas temperature measurements made at the gasifier exhaust. Samples 80-89 are estimated values. Tests 147-169, 199-203, 227-249, 262-284 are average values for each firing. All other temperatures measured during each test at the exit.
Velocity (meter/second)	Axial velocity component computed from input gas flow rates and primary/secondary geometries.
Momentum (kg/sq.-m*sec /kg/sq.-m*sec)	Momentum flux ratio in the axial direction computed from gas velocity multiplied by gas density.
(M1-M2)/Min (kg/sec / kg/sec, or DF)	<p>Particle-gas discrepancy factor.</p> <p>Definitions:</p> <p>M1 = gas mass flow rate out of the reactor calculated from the gas phase concentration measurements using local mass balance considerations and assuming a flat mass flux profile at the exit</p> <p>M2 = gas mass flow rate out of the reactor calculated from the particle phase (char) composition measurements and assuming a flat mass flux profile at the exit</p> <p>Min = total mass entering the reaction chamber</p>
Pollutant Gas Analyses (ppm)	The tabulated measured species concentrations for NO, NH ₃ , HCN, H ₂ S, COS, CS ₂ , and SO ₂ were computed to be on a water free basis.

APPENDIX A
SUMMARY OF COAL TYPE PARAMETRIC VARIATION TESTS

TABLE A1 SUBTASK 1.1 PARAMETRIC VARIATION TEST MEASURED VALUES

COAL TYPE	TEST NO.	FLOWRATES, (KG/HR)				NORMALIZED WATER-FREE GAS ANALYSIS, (MOLE PERCENT)				CHAR ANALYSIS (WEIGHT %)			
		PRIMARY COAL	STREAM AR	WINDOW O ₂	PURGE	AR	CO	CO ₂	H ₂	CH ₄	O ₂	N ₂	C
N.D.	103	33.8	4.78	22.75	0.92	7.63	40.38	20.95	27.10	0.94	0.36	2.64	41.59
N.D.	104	29.2	4.81	25.54	0.92	9.44	28.46	41.62	17.19	0.14	0.00	3.15	22.72
N.D.	105	32.3	4.89	20.95	0.92	10.13	26.06	43.84	16.11	0.09	0.00	3.73	51.00
N.D.	106	43.2	8.76	22.40	1.02	10.48	39.15	21.18	26.03	0.32	0.08	2.35	15.57
N.D.	107	29.5	6.40	27.92	1.02	10.63	36.42	25.30	24.30	0.76	0.10	2.34	9.40
N.D.	108	32.5	6.56	24.99	1.02	11.35	26.44	42.25	18.79	0.55	0.00	2.42	2.69
N.D.	109	43.5	8.81	22.32	0.93	6.39	41.96	22.47	25.90	0.68	0.31	2.30	23.03
N.D.	110	28.2	3.37	23.09	0.93	7.49	32.72	37.03	19.22	0.21	0.00	3.33	11.74
N.D.	111	23.1	3.56	27.90	0.93	8.03	19.66	58.15	10.66	0.00	0.00	3.50	6.20
N.D.	112	38.6	4.00	27.61	0.93	7.42	33.91	37.51	18.09	0.00	0.39	2.68	3.84
N.D.	113	43.5	4.75	34.44	0.93	6.93	36.88	34.78	18.90	0.00	0.32	2.20	4.53
N.D.	114	43.5	5.40	39.05	0.92	6.44	30.50	48.74	11.43	0.00	0.45	2.44	2.01
N.D.	115	43.5	5.37	31.04	0.92	6.44	37.57	37.34	16.28	0.00	0.00	2.37	15.14
N.D.	116	43.5	5.36	38.40	0.93	6.22	36.43	39.64	15.73	0.00	0.24	2.24	5.01
N.D.	117	53.0	5.38	34.22	0.99	5.45	41.02	25.75	25.77	0.24	0.00	1.77	6.58
N.D.	118	53.0	5.42	42.20	0.99	6.08	39.73	29.70	22.92	0.00	0.00	1.57	13.58
N.D.	119	53.0	5.44	34.96	0.99	5.99	41.68	26.35	24.02	0.00	0.00	1.96	9.16
N.D.	120	31.5	4.75	27.49	0.99	9.19	33.50	33.47	20.41	0.00	0.44	2.99	2.33
WYO.	34	31.1	5.71	17.35	0.36	6.31	50.42	13.29	28.88	0.93	0.12	0.05	35.52
WYO.	35	31.1	5.71	30.91	0.37	5.95	49.68	11.20	29.22	0.99	0.00	0.06	30.88
WYO.	36	31.1	5.73	24.58	0.37	5.78	48.63	18.28	26.87	0.17	0.00	0.07	18.25
WYO.	37	42.3	5.59	28.17	0.37	4.89	49.08	16.48	27.08	0.20	0.00	0.26	19.21
WYO.	38	42.3	5.60	25.05	0.36	4.12	52.00	9.30	33.31	1.31	0.00	-0.04	29.61
WYO.	39	111.0	24.01	62.65	0.27	4.99	22.43	52.09	12.66	0.43	7.81	-4.1	31.67
WYO.	40	111.0	23.77	73.75	0.27	6.52	51.28	12.97	29.24	0.22	0.00	-0.23	14.64
WYO.	41	34.5	5.66	32.64	0.37	6.44	40.36	31.34	18.71	0.00	0.00	0.00	3.64
WYO.	42	43.0	5.66	38.40	0.38	5.39	49.49	12.96	27.92	0.00	0.00	0.25	3.15
WYO.	43	87.5	9.58	55.51	0.67	11.02	49.97	9.09	25.32	0.54	0.00	1.07	21.03
WYO.	44	85.2	11.36	55.17	0.13	10.72	51.23	8.02	28.34	0.83	0.00	0.30	32.58
WYO.	45	66.7	7.86	58.94	0.13	10.28	51.35	13.60	23.54	0.00	0.00	0.56	19.85
WYO.	46	65.7	7.87	69.09	0.13	10.93	48.69	23.61	15.39	0.00	0.00	0.68	12.30
WYO.	47	65.7	7.79	69.90	0.13	10.10	49.23	22.41	16.84	0.00	0.00	0.66	4.90
WYO.	48	31.0	6.45	23.60	1.34	4.91	50.16	13.96	27.92	0.14	0.00	2.2	34.23
WYO.	49	31.0	6.43	27.08	1.33	4.40	56.44	13.77	25.95	0.00	0.00	1.3	18.91
WYO.	50	31.0	6.43	27.08	1.33	5.47	51.62	14.92	25.34	0.20	0.00	2.45	16.99
WYO.	51	28.0	10.17	23.43	1.33	6.99	46.55	20.32	23.46	0.00	0.00	2.69	4.88
WYO.	52	28.0	9.82	27.83	1.33	7.22	45.57	22.04	22.55	0.00	0.00	2.61	3.56
WYO.	53	28.0	9.75	23.55	1.33	6.81	48.92	16.84	24.93	0.00	0.00	2.50	7.47
WYO.	54	67.2	7.94	34.67	1.27	3.50	51.30	11.55	30.33	1.96	0.05	1.30	57.74
WYO.	55	58.8	8.42	42.17	1.28	3.48	52.41	13.96	27.95	0.14	0.00	2.2	31.89
WYO.	56	51.0	7.95	34.97	1.28	3.58	51.75	12.79	29.12	1.21	0.01	1.54	62.11
WYO.	57	52.5	7.90	42.12	1.27	4.67	49.83	16.09	27.31	0.52	0.00	1.59	55.53
WYO.	58	46.7	12.59	34.97	1.27	9.37	47.99	14.27	25.73	0.85	0.00	1.28	46.89
WYO.	59	33.4	12.74	42.43	1.28	15.77	32.85	31.18	12.44	0.29	4.97	2.49	30.72
WYO.	60	49.4	11.43	34.79	1.28	5.97	52.35	10.50	29.43	0.97	0.00	0.78	60.83
WYO.	61	52.9	11.38	42.40	1.28	5.19	51.90	13.81	27.57	0.35	0.00	1.18	50.45
WYO.	62	46.7	11.43	42.22	1.28	5.48	50.44	16.84	27.52	0.39	0.00	1.51	34.79
WYO.	63	52.2	11.43	34.82	1.28	5.13	50.92	14.92	27.47	0.07	0.00	1.49	32.11
ILL.	93	40.1	4.01	22.31	1.13	4.62	53.35	7.76	30.73	1.09	0.02	1.94	58.75
ILL.	94	33.8	4.06	27.89	1.18	4.42	55.79	12.59	24.87	0.05	0.00	2.27	47.05
ILL.	95	33.8	4.02	27.63	1.19	4.44	55.72	12.52	24.96	0.05	0.00	2.32	45.27
ILL.	96	33.8	4.02	22.92	1.19	4.43	56.38	8.36	28.06	0.35	0.00	2.23	40.11
ILL.	97	30.7	5.21	22.51	1.27	4.40	56.44	13.77	25.95	0.00	0.00	1.3	18.91
ILL.	98	41.3	5.07	27.99	1.27	4.96	56.93	7.00	28.82	0.12	0.00	2.17	37.30
ILL.	99	41.3	5.07	27.95	1.27	4.66	57.05	7.21	29.04	0.09	0.00	1.95	42.58
ILL.	100	50.6	4.96	33.92	1.19	3.71	58.32	6.80	29.43	0.21	0.02	1.50	44.88
ILL.	101	50.6	4.95	42.17	1.19	3.11	58.54	11.84	25.01	0.00	0.00	1.49	35.96
ILL.	102	50.6	4.94	34.43	1.19	3.20	58.17	9.95	26.63	0.02	0.12	1.91	36.77

TABLE A2 SUBTASK 1.1 PARAMETRIC VARIATION TEST COMPUTED VALUES

COAL TYPE	TEST NO.	PROBE LOC. (CM)	RATIOS (KG/KG)			PRES-SURE (ATM)	GAS MOL % O ₂	NM GAS (DRY)	CONVERSION % BASIS:					MIXING AND REACTION PARAMETERS				VISCOSITY (cP)	Re		
			O ₂ /COAL	H ₂ O/COAL	H ₂ O/O ₂				C	H	ASH, O	DRY N	FOR TOT S	TOT	ETA	GAM	F			ADJ. ETA	
N.D.	103	173	0	0.67	0.40	1.2	5.3	34.46	25.21	87.92	98.10	99.99	91.95	0.00	81.75	0.49	0.05	1.00	0.51	405.7	1793.
N.D.	104	173	0	0.87	0.40	1.2	5.2	35.17	31.33	95.23	98.49	99.99	96.88	25.18	86.80	0.45	0.04	1.00	0.46	412.7	1807.
N.D.	105	173	0	0.65	0.41	1.0	5.6	35.70	32.06	80.51	97.17	99.57	87.64	0.00	76.04	0.46	0.05	1.00	0.48	414.3	1369.
N.D.	106*	173	0	0.52	0.40	0.8	9.2	25.87	25.82	96.96	98.94	99.99	88.65	0.00	87.77	0.51	0.04	1.00	0.52	392.1	2367.
N.D.	107	173	0	0.95	0.40	1.4	8.6	35.77	27.07	98.27	98.21	99.99	98.36	0.00	88.40	0.46	0.04	1.00	0.46	416.8	1831.
N.D.	108	173	0	0.70	0.40	0.9	9.2	27.08	31.85	99.55	99.06	99.99	99.83	49.77	89.66	0.43	0.03	1.00	0.44	1831.	2262.
N.D.	109*	173	0	0.54	0.39	1.1	5.3	30.86	25.58	94.97	98.15	99.99	95.99	4.20	86.26	0.51	0.04	1.00	0.52	399.7	2300.
N.D.	110	173	0	0.82	0.39	1.2	4.9	31.58	29.82	97.76	98.54	99.99	97.85	0.00	97.96	0.47	0.04	1.00	0.48	407.4	1720.
N.D.	111*	173	0	1.21	0.38	1.4	4.9	36.04	35.45	98.92	98.66	99.99	97.21	38.45	89.10	0.42	0.03	1.00	0.42	414.8	1695.
N.D.	112	173	0	0.71	0.39	1.1	5.0	32.16	30.23	99.33	98.44	99.99	98.15	14.65	89.13	0.46	0.03	1.00	0.47	422.4	2254.
N.D.	113	173	0	0.79	0.39	1.1	5.3	30.93	29.52	99.20	98.37	98.83	96.83	16.02	88.77	0.46	0.03	1.00	0.47	423.5	2569.
N.D.	114	173	0	0.90	0.38	1.0	4.9	31.28	33.63	99.68	98.59	99.99	99.28	70.23	90.27	0.48	0.03	1.00	0.48	441.4	2481.
N.D.	115	173	0	0.71	0.39	0.8	4.9	26.43	30.53	96.97	93.32	99.99	96.41	78.73	87.43	0.51	0.03	1.00	0.51	437.2	2475.
N.D.	116	173	0	0.88	0.39	1.0	5.0	29.51	31.16	99.15	98.21	99.99	98.40	67.31	89.36	0.48	0.03	1.00	0.48	437.2	2475.
N.D.	117	173	0	0.65	0.40	0.7	9.9	20.71	26.07	98.87	98.65	99.99	97.81	23.45	89.04	0.51	0.03	1.00	0.52	393.0	2924.
N.D.	118	173	0	0.80	0.40	1.1	9.9	31.63	27.48	97.31	97.98	98.87	98.35	11.06	87.54	0.50	0.02	1.00	0.51	440.1	2740.
N.D.	119	173	0	0.66	0.40	0.8	9.7	23.12	26.73	98.29	98.12	98.39	97.53	36.16	88.29	0.49	0.03	1.00	0.49	419.2	2910.
N.D.	120	173	0	0.87	0.39	1.3	9.7	34.03	29.20	98.62	98.85	99.99	98.51	54.46	89.78	0.46	0.04	1.00	0.47	423.3	1922.
WYO.	34*	173	0	0.56	0.30	0.6	5.6	14.92	23.26	93.92	99.73	99.44	96.41	55.84	88.17	0.59	0.01	1.00	0.59	374.7	1612.
WYO.	35	173	0	0.67	0.31	0.6	5.6	13.74	23.26	95.31	99.78	99.97	95.99	72.60	89.28	0.58	0.00	1.00	0.58	176.1	1728.
WYO.	36	173	0	0.80	0.30	0.7	5.6	16.90	24.57	97.60	99.80	99.99	98.65	76.57	90.90	0.55	0.00	1.00	0.55	392.5	1785.
WYO.	37	173	0	0.67	0.30	0.7	5.6	17.51	24.48	97.47	99.80	99.94	97.74	81.57	90.84	0.57	0.00	1.00	0.57	406.7	2210.
WYO.	38*	173	0	0.59	0.30	0.3	5.6	8.49	21.19	95.60	99.54	99.99	98.07	82.09	89.66	0.61	0.00	1.00	0.61	380.6	2097.
WYO.	39*	173	0	0.56	0.30	1.0	10.2	31.71	33.56	94.95	99.77	99.41	94.27	64.29	88.92	0.56	0.20	1.00	0.61	492.4	4623.
WYO.	40	173	0	0.66	0.30	0.6	10.2	33.45	23.17	98.17	99.87	99.99	98.39	80.03	91.37	0.58	0.00	1.00	0.58	422.4	5509.
WYO.	41	173	0	0.95	0.22	1.2	5.6	23.55	28.44	99.49	99.99	99.99	99.99	99.99	99.99	0.58	0.00	1.00	0.58	408.8	2043.
WYO.	42	173	0	0.75	0.28	0.9	5.6	16.95	23.97	99.45	99.80	99.99	99.28	88.46	92.33	0.55	0.00	1.00	0.55	411.3	3401.
WYO.	43	173	0	0.63	0.28	2.1	5.8	38.15	23.32	97.13	99.56	99.99	98.58	61.32	90.50	0.41	0.03	1.00	0.42	492.1	4462.
WYO.	44	173	0	0.65	0.26	2.5	5.7	40.04	22.97	94.86	99.22	99.99	96.82	21.28	89.07	0.45	0.01	1.00	0.46	487.6	4692.
WYO.	45	173	0	0.88	0.26	3.0	5.7	44.43	25.14	97.30	99.62	99.85	98.43	52.42	90.56	0.43	0.01	1.00	0.43	525.4	3729.
WYO.	46	173	0	1.05	0.26	3.4	5.6	49.99	29.16	98.49	99.67	99.99	98.65	74.63	91.55	0.40	0.01	1.00	0.40	550.9	3643.
WYO.	47	173	0	1.06	0.26	3.3	5.7	48.47	28.25	99.46	99.91	99.99	98.74	92.92	92.34	0.40	0.01	1.00	0.40	556.3	3809.
WYO.	48	173	0	0.76	0.20	0.8	5.6	12.10	23.41	94.27	99.04	99.99	96.17	18.44	87.46	0.51	0.00	1.00	0.51	355.1	2075.
WYO.	49	173	0	0.83	0.21	0.8	5.8	11.90	24.44	97.82	99.61	99.99	97.96	41.40	91.15	0.52	0.06	1.00	0.54	359.4	2285.
WYO.	50	173	0	0.84	0.20	1.1	10.0	16.27	25.98	99.43	99.79	98.30	98.90	63.44	91.82	0.50	0.14	1.00	0.54	372.0	2114.
WYO.	52	173	0	0.99	0.21	1.2	9.9	17.30	26.52	99.59	99.65	99.99	99.56	46.16	92.31	0.50	0.11	1.00	0.52	380.8	2179.
WYO.	53	173	0	0.84	0.21	1.0	10.0	14.62	25.01	99.15	99.57	99.99	99.02	67.00	92.12	0.52	0.12	1.00	0.55	371.6	2072.
WYO.	54*	173	0	0.52	0.20	0.7	5.6	12.09	22.16	85.52	98.08	99.99	86.94	7.70	82.99	0.59	0.10	1.00	0.62	355.5	3758.
WYO.	55	173	0	0.68	0.20	1.0	5.6	17.33	23.26	85.64	97.77	99.99	89.01	0.00	82.24	0.59	0.10	1.00	0.62	377.3	3309.
WYO.	56	173	0	0.72	0.20	0.9	5.3	15.99	22.79	88.13	96.95	99.99	98.81	69.17	87.46	0.58	0.11	1.00	0.59	370.5	3809.
WYO.	57	173	0	0.80	0.20	0.7	5.6	10.00	22.00	88.13	97.95	99.99	90.91	0.00	82.71	0.52	0.03	1.00	0.53	369.6	3406.
WYO.	58	173	0	0.75	0.20	1.0	10.0	13.52	24.65	90.65	98.94	99.99	94.78	14.93	86.19	0.47	0.03	1.00	0.48	372.4	1463.
WYO.	59*	173	0	1.27	0.20	2.7	10.4	29.76	31.77	95.34	99.12	99.99	95.78	61.70	89.45	0.34	0.02	1.00	0.35	422.2	3194.
WYO.	60	173	0	0.70	0.22	0.4	10.1	6.97	22.58	83.93	97.63	99.99	88.50	18.14	81.64	0.56	0.03	1.00	0.57	354.6	1013.
WYO.	61	173	0	0.80	0.22	0.8	10.0	13.35	23.61	89.07	98.20	99.99	94.10	47.34	84.94	0.55	0.07	1.00	0.57	376.1	3230.
WYO.	62	173	0	0.87	0.22	0.8	10.2	13.55	24.35	94.25	99.09	99.99	95.11	57.59	88.52	0.54	0.07	1.00	0.56	384.0	3149.
WYO.	63	173	0	0.67	0.22	0.9	10.2	14.52	23.84	95.00	99.00	99.99	97.31	60.00	89.20	0.55	0.11	1.00	0.58	382.7	3176.
ILL.	93*	173	0	0.56	0.10	1.2	5.5	10.83	22.00	69.59	97.35	99.99	84.68	60.08	65.98	0.51	0.06	1.00	0.53	350.2	2355.
ILL.	94	173	0	0.23	0.10	1.3	5.4	11.57	24.46	81.29	98.24	99.99	90.43	69.00	73.76	0.49	0.04	1.00	0.50	357.3	2352.
ILL.	95	173	0	0.82	0.10	1.4	5.3	11.32	24.42	82.91	98.59	99.99	88.81	65.63	75.11	0.49	0.04	1.00	0.50	356.8	2420.
ILL.	96	173	0	0.65	0.10	1.0	5.4	7.34	22.83	86.35	98.39	99.99	90.69	69.59	77.56	0.51	0.05	1.00	0.52	344.2	2403.
ILL.	97	173	0	0.76	0.10	0.6	10.1	5.41	22.58	85.16	99.06	99.99	92.76	68.15	76.54	0.55	0.07	1.00	0.56	342.2	2093.
ILL.	98	173	0	0.68	0.10	1.0	9.9	8.30	22.49	87.54	95.98	99.99	94.44	69.17	77.94	0.52	0.09	1.00	0.52	351.1	2891.
ILL.	99	173	0	0.68	0.10	0.9	9.6	7.75	22.44	88.14	97.21	99.99	92.29	68.15	76.63	0.53	0.04	1.00	0.52	351.3	2805.
ILL.	100	173	0	0.57	0.10	1.0	10.2	7.14	21.41	87.17	97.17	99.99	92.02	67.45	75.37	0.53	0.03	1.00	0.54	358.3	3251.
ILL.	101	173	0	0.33	0.10	1.0	5.4	8.98	24.02	88.51	95.59	99.99	92.12	69.92	78.96	0.52	0.03	1.00	0.53	376.2	3311.
ILL.	102	173	0	0.68	0.10	0.9	6.4	8.19	23.28	87.85	99.62	99.99	92.41	65.94	78.17	0.55	0.06	1.00	0.56	365.2	3331.

TABLE A2 SUBTASK 1.1 PARAMETRIC VARIATION TEST COMPUTED VALUES (CONTINUED)

COAL TYPE	TEST NO.	ELEMENTAL CLOSURES										MASS OUT (KG)/MASS IN (KG)										ENERGY BALANCE (OUT/IN)					OUTLET TEMP. (K)	VELOCITY (M/S)	(M1-M2) /Min																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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		C	H	O	N	S	Az	C	H	O	N	S	Az	TOT	GAS	CHAR	GAS	CHAR	LOST																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									

APPENDIX B
SUMMARY OF COAL TYPE MAPPING TESTS

TABLE B1 SUBTASK 1.1 MAPPING TEST MEASURED VALUES

COAL TYPE	TEST NO.	FLOWRATES (KG/HR)					NORMALIZED WATER-FREE GAS ANALYSIS (MOLE PERCENT)							CHAR ANALYSIS (WEIGHT %)					
		PRIMARY COAL	STREAM AR	WINDOW O2	PURGE	AR	CO	CO2	R2	CH4	O2	N2	C	H	O	N	S	ASH	
N.D.	328	22.4	5.40	27.92	1.35	16.03	22.39	50.16	8.96	0.00	2.07	0.19	5.64	0.24	10.58	0.08	1.32	82.14	
N.D.	329	22.1	5.54	28.08	1.37	13.03	28.38	49.72	7.82	0.00	0.65	0.41	4.66	0.40	8.43	0.11	0.62	85.78	
N.D.	330	26.9	5.23	28.00	1.37	11.58	24.77	56.94	6.28	0.00	0.00	0.44	3.14	0.88	3.58	0.10	0.39	91.91	
N.D.	331	37.3	5.45	28.00	1.37	9.96	35.62	43.41	10.59	0.00	0.00	0.42	1.17	0.17	4.99	0.00	0.50	93.17	
N.D.	332	37.3	5.45	27.92	1.37	7.88	47.17	24.66	20.11	0.00	0.00	0.18	8.50	0.14	5.72	0.09	2.59	82.96	
N.D.	333	37.3	5.44	27.92	1.37	7.14	42.52	26.41	20.47	0.11	0.00	0.05	1.44	0.11	5.10	0.16	3.81	83.91	
N.D.	334	39.0	6.12	27.92	1.38	10.44	42.52	26.41	20.47	0.11	0.00	0.05	7.90	0.05	10.27	0.26	2.79	78.73	
N.D.	336	34.8	6.21	28.17	1.39	10.91	38.67	33.77	15.10	0.00	0.21	0.34	1.44	0.11	0.89	0.33	2.99	89.38	
N.D.	338	34.1	6.31	28.08	1.39	9.92	36.73	35.56	15.10	0.00	2.40	0.29	7.01	0.01	2.57	0.13	2.88	92.87	
N.D.	339	34.1	6.27	28.08	1.39	9.89	40.42	31.66	17.69	0.02	0.00	0.32	11.10	0.00	9.60	0.42	4.44	81.81	
N.D.	340	34.1	6.25	28.00	1.39	10.33	41.74	29.66	17.95	0.00	0.00	0.32	20.51	0.19	12.53	0.46	3.45	62.76	
N.D.	341	34.1	6.26	28.00	1.39	10.27	42.18	29.41	17.05	0.00	0.75	0.35	27.33	0.16	-0.96	0.44	2.64	70.39	
N.D.	343	35.1	6.67	27.83	1.40	7.72	46.91	19.94	24.68	0.15	0.40	0.19	11.24	0.01	2.14	0.25	4.90	81.46	
N.D.	344	35.1	6.47	28.00	1.40	9.07	42.95	25.83	21.76	0.09	0.00	0.31	5.55	0.14	4.28	0.13	1.72	88.18	
N.D.	345	35.1	6.86	28.08	1.41	10.77	33.44	39.75	15.63	0.00	0.00	0.40	6.62	0.00	6.37	0.12	2.70	84.19	
N.D.	346	35.1	6.84	28.16	1.40	10.07	40.30	31.77	17.53	0.00	0.00	0.33	5.50	0.00	4.14	0.20	4.17	85.99	
N.D.	347	32.0	6.09	28.41	1.30	10.31	36.85	33.98	17.90	0.00	1.05	0.30	1.13	0.08	-3.52	0.13	5.64	96.54	
N.D.	348	32.0	6.10	27.83	1.35	11.42	36.38	34.54	15.75	0.00	0.00	0.43	0.73	0.00	7.96	0.24	1.73	89.08	
N.D.	349	32.0	6.19	27.83	1.33	12.75	32.41	41.45	13.01	0.00	0.00	0.38	0.88	0.11	7.96	0.19	3.21	87.97	
N.D.	350	32.0	6.17	27.91	1.33	11.13	34.66	39.66	13.14	0.00	1.04	0.38	1.06	0.04	7.83	0.10	3.59	88.68	
N.D.	352	30.5	6.69	27.83	1.36	16.73	16.46	46.56	6.18	0.00	3.69	0.38	0.66	0.07	5.64	0.11	1.21	92.31	
N.D.	353	30.5	6.70	27.83	1.36	13.84	30.34	42.00	12.20	0.00	1.30	0.33	0.38	0.08	5.42	0.06	2.83	91.23	
N.D.	354	30.5	6.69	27.99	1.40	13.57	30.95	42.16	12.35	0.00	0.58	0.39	0.39	0.06	5.55	0.22	1.17	92.61	
WYO.	285	50.0	4.81	27.92	1.37	4.98	52.98	12.16	27.98	1.69	0.25	-0.04	62.85	0.22	-3.57	0.42	2.63	37.45	
WYO.	286	50.7	5.01	27.92	1.35	5.08	54.20	10.81	28.41	1.42	0.00	0.07	57.03	0.00	-3.43	0.60	2.36	43.44	
WYO.	287	50.7	5.18	27.92	1.38	4.77	55.14	10.94	29.58	1.23	0.00	0.02	53.92	0.18	-2.31	0.48	2.60	45.13	
WYO.	289	50.7	5.18	28.08	1.39	4.90	53.73	9.48	29.58	2.23	0.00	-0.32	66.74	0.00	-2.46	0.68	2.52	32.52	
WYO.	290	50.7	5.18	27.92	1.36	4.66	54.02	9.60	29.84	2.19	0.00	-0.32	68.70	0.21	-3.38	0.63	2.17	30.67	
WYO.	291	17.1	3.42	28.00	1.36	6.91	52.57	13.91	25.21	1.17	0.00	0.22	62.43	0.44	-0.31	0.64	1.58	35.22	
WYO.	292	17.1	3.40	28.00	1.37	4.67	54.35	17.91	22.44	0.33	0.00	0.29	49.20	0.46	1.22	0.51	1.51	47.10	
WYO.	293	17.1	3.44	27.92	1.37	6.12	52.70	18.42	20.25	0.20	2.00	0.31	37.32	0.39	8.13	0.48	1.81	51.87	
WYO.	294	17.1	3.42	28.08	1.37	6.06	54.80	17.11	21.49	0.21	0.00	0.32	40.87	0.44	0.16	0.39	2.20	55.94	
WYO.	295	17.1	3.45	27.92	1.37	7.33	51.06	24.07	17.11	0.02	0.00	0.41	29.13	0.08	2.63	0.33	1.55	66.28	
WYO.	296	33.2	4.44	27.91	1.39	5.34	54.15	11.12	27.90	1.32	0.06	-0.10	53.72	0.05	-1.01	0.44	1.66	43.14	
WYO.	297	33.2	4.37	27.66	1.39	5.79	53.84	10.72	28.24	1.17	0.00	0.23	55.30	0.27	-2.76	0.66	1.65	44.88	
WYO.	298	33.2	4.36	27.74	1.40	5.79	53.84	10.72	28.24	1.17	0.00	0.23	57.12	0.00	-3.01	0.32	2.32	57.23	
WYO.	299	23.9	4.47	27.74	1.40	8.40	48.12	23.61	18.94	0.11	0.00	0.43	25.60	0.28	0.54	0.24	1.01	72.33	
WYO.	300	23.9	4.72	27.83	1.41	10.33	40.56	35.38	13.18	0.00	0.91	0.43	18.15	0.13	7.49	0.24	0.41	71.66	
WYO.	301	39.5	3.99	27.82	1.45	3.85	51.93	10.62	31.48	2.61	0.03	-0.52	70.92	0.07	5.77	0.59	1.57	21.08	
WYO.	302	39.5	4.17	27.74	1.49	4.93	51.38	11.35	30.38	1.82	0.68	-0.36	50.18	0.87	11.17	0.42	1.49	36.66	
WYO.	303	39.5	4.49	27.98	1.44	4.68	53.35	13.12	28.03	0.85	0.00	-0.02	36.30	0.20	21.04	0.46	1.80	40.20	
WYO.	304	39.5	4.47	27.82	1.47	5.14	53.80	14.35	26.10	0.46	0.00	-0.16	35.83	0.04	7.26	0.36	2.13	54.38	
WYO.	305	19.5	4.48	27.82	1.49	8.37	52.79	13.37	26.55	1.07	2.00	-0.16	51.86	0.12	2.76	0.47	2.11	42.68	
WYO.	308	30.7	4.87	27.83	1.30	7.07	50.63	15.73	25.57	0.79	0.00	0.21	47.57	0.15	2.14	0.46	2.95	46.52	
WYO.	308	30.7	4.87	28.08	1.35	7.58	50.91	20.31	20.77	0.13	0.00	0.30	23.43	0.17	6.97	0.43	2.48	66.52	
WYO.	309	39.9	4.75	27.91	1.39	6.07	52.38	14.57	26.01	0.86	0.00	0.11	46.75	0.48	22.08	0.46	1.73	28.50	
WYO.	310	39.9	4.76	27.83	1.29	6.83	50.98	21.56	20.09	0.33	0.00	0.22	61.23	1.60	11.47	0.77	0.84	24.09	
WYO.	312	29.4	5.84	27.83	1.42	8.02	52.86	13.58	25.11	0.42	0.00	0.02	38.88	0.51	5.68	0.37	0.32	52.53	
WYO.	313	18.6	6.03	27.91	1.43	9.68	50.05	19.45	19.48	0.11	0.94	0.29	26.54	0.23	10.79	0.28	1.59	60.57	
WYO.	314	27.7	6.10	27.99	1.44	7.99	51.79	19.35	20.70	0.01	0.00	0.15	18.48	0.33	4.75	0.19	1.91	74.34	
WYO.	315	32.5	6.01	27.99	1.44	7.85	52.55	16.40	22.89	0.13	0.00	0.18	25.20	0.20	1.08	0.31	2.23	70.98	
WYO.	316	32.5	5.90	27.91	1.45	9.15	52.35	15.92	22.27	0.16	0.00	0.14	34.41	0.16	5.47	0.46	1.69	57.79	
WYO.	317	32.5	5.91	27.91	1.46	8.50	49.50	21.07	18.47	0.07	2.26	0.13	40.51	0.35	9.81	0.72	0.85	47.76	
WYO.	318	31.5	4.61	28.00	1.33	5.88	51.98	14.13	26.88	1.13	0.00	-0.01	48.10	0.36	-1.16	0.46	2.11	50.13	
WYO.	319	31.5	4.62	27.92	1.34	6.75	51.48	17.11	24.02	0.60	0.00	0.05	36.08	0.23	7.73	0.48	2.04	53.44	
WYO.	320	31.5	4.65	27.96	1.35	8.70	45.73	28.74	15.12	0.00	1.45	0.26	19.57	0.28	1.75	0.20	1.68	76.52	
WYO.	322	31.5	4.61	27.92	1.37	6.08	52.73	13.55	27.90	0.99	0.00	-0.15	52.42	0.57	2.75	0.49	1.46	42.11	
WYO.	323	29.6	4.64	27.92	1.38	8.24	45.90	24.31	18.27	0.10	0.00	0.18	19.12	0.24	17.08	0.29	1.46	61.07	
WYO.	325	35.5	4.35	27.92	1.40	5.86	52.79	15.92	25.26	0.39	0.00	-0.22	37.81	0.39	-12.19	0.51	1.75	71.73	
WYO.	326	35.5	4.36	27.92	1.40	5.07	53.93	15.03	25.70	0.55	0.00	-0.28	25.63	0.24	2.91	0.25	1.61	69.16	
WYO.	327	35.5	4.33	27.84	1.40	4.84	54.01	15.67	25.36	0.39	0.00	-0.27	14.97	0.14	10.39	0.14	1.60	72.76	
ILL.	362	34.5	5.43	28.00	1.38	7.09	55.56	10.86	24.21	0.09	1.72	0.47	32.62	0.17	-1.39	0.30	5.97	62.33	
ILL.	363	34.5	5.43	27.83	1.39	6.87	57.04	10.80	23.36	0.05	1.40	0.48	31.54	0.14	-0.08	0.28	5.69	62.43	
ILL.	364	38.9	5.29	27.96	1.39	6.76	57.98	11.16	23.61	0.00	0.00	0.49	29.04	0.12	1.16	0.27	3.48	65.93	
ILL.	365	30.9	5.28	28.00	1.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	44.15	0.00	0.10	0.39	3.36	43.80	
ILL.	366	36.9	5.28	28.12	1.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	55.13	0.20	5.41	0.46	3.64	35.16	
ILL.	367	50.4	6.73	42.13	1.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00	45.23	0.24	-3.31	0.58			

TABLE B2 SUBTASK 1.1 MAPPING TEST COMPUTED VALUES

COAL TYPE	TEST NO.	PROBE LOC (CM)	RATIOS (KG/KG)		PRES- SURE (ATM)	GAS MOL % H ₂	MW GAS (DRY)	CONVERSION % BASIS:					MIXING AND REACTION PARAMETERS					
			O ₂ / COAL	H ₂ O/ H ₂ O (O/I)				C	H	ASH, O	(NAT FOR TOT) N	S	TOT	ETA	GAM	F	ADJ.	ETA
N.D.	323	83, 8	1.25	0.37	1.0	5.3	31.10	35.69	98.94	99.33	94.23	98.95	81.44	88.19	0.41	0.07	1.00	0.43
N.D.	329	83, 8	1.22	0.37	1.0	5.5	32.69	35.51	99.16	98.93	95.60	98.62	91.65	88.69	0.42	0.05	1.00	0.44
N.D.	330	83, 6	1.04	0.37	1.0	5.7	34.36	36.86	99.47	97.79	98.26	98.83	95.10	89.45	0.43	0.02	1.00	0.43
N.D.	331	83, 4	0.75	0.37	1.0	5.8	31.84	33.39	99.81	99.58	97.60	99.99	93.80	89.59	0.46	0.01	1.00	0.46
N.D.	332	83, 2	0.75	0.37	1.0	5.7	24.37	27.45	98.41	99.61	96.91	98.83	63.95	88.31	0.52	0.04	1.00	0.53
N.D.	333	83, 0	0.75	0.37	1.0	5.7	24.53	27.73	98.45	99.85	94.16	96.44	59.08	87.68	0.52	0.01	1.00	0.52
N.D.	334	83, 8	0.72	0.37	1.0	9.6	23.58	28.10	98.29	99.64	99.99	94.50	61.37	89.15	0.51	0.04	1.00	0.53
N.D.	336	83, 6	0.81	0.37	1.0	9.7	27.35	30.34	99.76	99.73	98.76	98.44	64.19	89.56	0.47	0.04	1.00	0.48
N.D.	338	83, 6	0.82	0.37	1.0	5.5	27.60	31.03	98.71	99.97	97.28	97.94	47.57	88.44	0.46	0.01	1.00	0.46
N.D.	339	83, 4	0.82	0.37	1.0	5.4	26.32	29.65	97.70	99.99	94.32	93.95	35.63	87.03	0.48	0.03	1.00	0.49
N.D.	340	83, 2	0.82	0.37	1.0	5.4	26.51	29.32	94.94	99.30	90.99	92.10	36.52	84.54	0.48	0.05	1.00	0.49
N.D.	341	83, 0	0.82	0.37	1.0	5.4	28.58	29.53	93.99	99.48	99.99	93.26	56.69	86.22	0.49	0.04	1.00	0.50
N.D.	343	83, 6	0.79	0.37	1.0	10.1	20.00	25.68	97.86	99.97	98.82	96.69	30.54	88.09	0.54	0.04	1.00	0.55
N.D.	344	83, 4	0.80	0.37	1.0	10.3	22.17	27.57	99.03	99.63	97.83	98.41	77.48	89.00	0.51	0.05	1.00	0.52
N.D.	345	83, 2	0.80	0.37	1.0	9.8	27.81	31.60	98.78	99.99	96.61	98.46	62.97	88.48	0.46	0.01	1.00	0.46
N.D.	346	83, 0	0.80	0.37	1.0	10.0	26.28	29.73	99.01	99.99	97.84	97.49	44.00	88.72	0.48	0.02	1.00	0.49
N.D.	347	22, 8	0.89	0.37	1.0	5.5	25.47	30.16	99.82	99.81	99.99	98.55	32.54	89.95	0.48	0.05	1.00	0.49
N.D.	348	22, 6	0.87	0.37	1.0	5.4	26.18	30.87	99.87	99.99	95.98	97.67	57.86	88.97	0.46	0.06	1.00	0.47
N.D.	349	22, 4	0.87	0.37	1.0	5.2	28.63	32.79	99.85	99.72	96.00	97.10	77.57	89.11	0.45	0.06	1.00	0.46
N.D.	351	22, 4	0.87	0.37	1.0	5.6	28.83	32.32	99.82	99.90	96.05	98.78	70.13	89.06	0.45	0.03	1.00	0.46
N.D.	352	22, 8	0.91	0.37	1.0	10.0	11.87	37.58	99.89	99.83	97.27	98.72	84.86	89.49	0.38	0.05	1.00	0.40
N.D.	353	22, 6	0.91	0.37	1.0	10.0	28.61	33.25	99.94	99.80	97.34	99.29	64.13	89.37	0.43	0.06	1.00	0.45
N.D.	354	22, 4	0.92	0.37	1.0	10.2	28.90	33.20	99.93	99.85	97.32	97.44	85.41	89.53	0.44	0.05	1.00	0.45
WYO.	285	83, 8	0.56	0.21	1.0	10.0	11.59	23.07	82.25	99.11	99.99	91.69	0.00	80.40	0.55	0.04	1.00	0.56
WYO.	286	83, 8	0.91	0.21	1.0	9.9	13.01	22.79	86.11	99.99	99.99	89.76	0.00	83.10	0.54	0.02	1.00	0.55
WYO.	287	83, 6	0.91	0.21	1.0	10.2	13.42	22.92	87.36	99.40	99.99	92.11	0.00	83.74	0.54	0.00	1.00	0.54
WYO.	289	83, 2	0.91	0.21	1.1	10.1	14.54	22.18	78.29	99.69	99.99	84.50	0.00	77.43	0.55	0.04	1.00	0.56
WYO.	290	83, 0	0.91	0.21	1.0	10.0	15.12	22.05	76.31	98.97	99.99	84.77	0.00	76.07	0.56	0.03	1.00	0.56
WYO.	291	83, 0	1.64	0.21	1.0	5.2	15.45	24.37	81.25	98.12	99.99	86.53	3.15	79.16	0.51	0.11	1.00	0.54
WYO.	292	83, 2	1.64	0.21	1.0	5.6	20.15	25.57	88.95	98.53	98.89	91.97	30.79	84.42	0.50	0.02	1.00	0.50
WYO.	293	83, 4	1.63	0.21	1.0	5.2	19.47	26.49	92.39	98.87	93.26	93.14	24.67	85.85	0.46	0.04	1.00	0.47
WYO.	294	83, 4	1.64	0.21	1.0	5.5	23.16	25.85	92.27	98.81	99.99	94.83	15.10	86.88	0.47	0.03	1.00	0.48
WYO.	295	83, 2	1.63	0.21	1.0	5.3	27.55	28.29	95.35	99.82	98.29	96.31	49.51	88.93	0.44	0.03	1.00	0.45
WYO.	296	22, 8	0.84	0.21	1.0	5.5	13.13	23.03	86.34	99.83	99.99	92.44	16.93	82.99	0.54	0.05	1.00	0.55
WYO.	297	22, 8	0.83	0.21	1.0	5.3	13.49	22.95	86.97	99.09	99.99	89.10	20.63	83.65	0.53	0.06	1.00	0.55
WYO.	298	22, 6	0.84	0.21	1.0	5.2	21.47	25.81	93.14	99.99	97.74	95.85	12.49	87.17	0.46	0.04	1.00	0.47
WYO.	299	22, 4	1.16	0.21	1.0	5.2	24.50	27.92	96.26	99.42	99.68	97.54	69.85	89.85	0.44	0.04	1.00	0.45
WYO.	300	22, 2	1.16	0.21	1.0	5.3	24.90	31.73	97.32	99.73	94.31	97.51	86.73	89.74	0.40	0.04	1.00	0.41
WYO.	301	22, 8	0.70	0.21	1.0	9.9	21.30	21.61	64.42	99.50	88.24	79.25	0.00	65.18	0.55	0.05	1.00	0.56
WYO.	302	22, 6	0.70	0.21	1.0	10.3	8.32	22.08	85.52	99.71	86.91	91.30	12.26	79.98	0.55	0.02	1.00	0.56
WYO.	303	22, 4	0.71	0.21	1.0	10.3	10.08	23.30	90.45	99.25	97.51	91.30	12.26	79.98	0.51	0.02	1.00	0.56
WYO.	304	22, 2	0.70	0.21	1.0	10.5	13.72	24.06	93.03	99.89	94.26	95.09	15.44	86.50	0.51	0.02	1.00	0.51
WYO.	305	22, 6	0.70	0.21	1.1	10.2	12.69	23.88	87.15	99.58	97.22	91.84	0.00	82.80	0.52	0.04	1.00	0.53
WYO.	306	52, 8	0.91	0.21	1.0	5.4	17.78	24.63	89.19	99.51	97.84	92.67	0.00	84.23	0.49	0.04	1.00	0.50
WYO.	308	52, 4	0.91	0.21	1.0	5.3	18.10	26.76	96.27	99.61	95.50	95.21	19.51	88.97	0.46	0.04	1.00	0.47
WYO.	309	52, 2	0.70	0.21	1.0	5.5	14.56	24.20	82.65	97.46	66.71	88.03	0.00	74.25	0.48	0.03	1.00	0.43
WYO.	310	52, 0	0.70	0.21	1.0	5.6	24.91	27.01	73.12	89.99	79.54	76.30	24.72	69.53	0.45	0.00	1.00	0.45
WYO.	312	52, 8	0.95	0.21	1.0	10.0	13.77	24.54	92.17	98.54	95.35	94.78	16.57	86.03	0.49	0.05	1.00	0.51
WYO.	313	52, 6	1.50	0.21	1.0	9.6	18.35	27.25	95.37	99.43	92.34	96.57	43.33	87.88	0.44	0.05	1.00	0.45
WYO.	314	52, 6	1.01	0.21	1.0	10.5	17.47	26.66	97.37	99.33	97.25	98.11	44.33	90.13	0.46	0.02	1.00	0.47
WYO.	315	52, 4	0.86	0.21	1.0	10.0	15.67	25.60	96.25	99.58	99.35	96.76	32.18	89.66	0.48	0.04	1.00	0.49
WYO.	316	52, 2	0.86	0.21	1.0	9.7	16.85	25.83	93.70	99.58	95.93	94.10	36.87	87.30	0.47	0.05	1.00	0.48
WYO.	317	52, 0	0.86	0.21	1.1	9.6	20.57	27.64	91.03	98.90	91.17	88.82	61.58	84.63	0.44	0.01	1.00	0.44
WYO.	318	83, 8	0.89	0.21	1.0	5.5	15.18	23.83	89.85	98.92	99.99	93.20	9.13	85.36	0.51	0.03	1.00	0.52
WYO.	319	83, 6	0.89	0.21	1.0	5.3	14.91	25.22	92.86	99.35	93.78	93.34	17.59	86.26	0.49	0.05	1.00	0.50
WYO.	320	83, 4	0.94	0.21	1.0	5.4	22.67	29.75	97.30	99.45	99.02	98.06	22.60	90.41	0.43	0.03	1.00	0.43
WYO.	322	83, 2	0.89	0.21	1.0	5.4	16.88	24.12	86.37	97.96	97.19	87.85	25.15	82.57	0.50	0.03	1.00	0.51
WYO.	323	83, 0	0.94	0.21	1.0	5.6	19.55	28.10	96.74	99.42	88.17	96.54	58.26	88.17				

TABLE B2 SUBTASK 1.1 MAPPING TEST COMPUTED VALUES (CONTINUED)

COAL TYPE	TEST NO.	ELEMENTAL CLOSURES					EXIT TEMP (K)	VELOCITY (M/S) PRI.	NITROGEN AND SULFUR POLLUTANT SPECIES						(PPM) SO2	
		OBSERVED	CALCULATED	(MOL/MOL)	S	AR			COMPUTED CONCENTRATION	WATER FREE BASIS	CS2					
		C	H	O	N				NO	NH3	HCN	H2S	COS			
N.D.	328	1.06	1.00	1.02	1.02	0.9	1.10	1027.	63.5	257.0	484.0	31.7	2467.3	106.8	0.0	0.0
N.D.	329	1.09	1.00	1.03	0.98	1.0	1.00	1077.	61.7	107.7	286.9	18.0	3005.1	191.5	0.0	0.0
N.D.	330	1.08	1.00	1.03	0.99	0.6	1.00	1102.	58.9	129.0	222.1	12.8	2195.8	92.5	0.0	0.0
N.D.	331	1.08	1.00	1.03	0.99	1.0	1.00	1122.	58.6	72.7	512.7	15.4	3131.5	249.6	0.0	0.0
N.D.	332	1.08	1.00	1.04	0.99	1.8	1.00	1144.	59.1	20.8	4378.9	82.6	3650.0	296.6	0.0	0.0
N.D.	333	1.09	1.00	1.04	0.99	2.0	1.00	1136.	59.1	16.4	3968.5	214.4	3690.4	298.4	0.0	0.0
N.D.	334	1.08	1.00	1.03	0.99	1.8	1.12	1144.	35.8	14.2	6454.1	316.8	3524.7	177.0	0.0	0.0
N.D.	336	1.08	1.00	1.03	0.99	1.8	1.00	1158.	35.9	11.1	13127.7	1405.4	3755.0	240.9	0.0	0.0
N.D.	338	1.08	1.00	1.03	0.99	0.6	1.00	1022.	63.2	55.5	2159.3	30.2	719.5	212.1	0.0	0.0
N.D.	339	1.09	1.00	1.04	0.99	0.6	1.00	1022.	65.1	32.7	1299.7	24.3	453.7	208.2	0.0	0.0
N.D.	340	1.09	1.00	1.04	0.99	0.8	1.00	1027.	64.9	25.8	1240.1	36.3	741.0	211.9	0.0	0.0
N.D.	341	1.05	1.00	1.02	0.99	0.4	1.00	1033.	64.9	30.7	1250.4	43.5	621.9	245.0	0.0	0.0
N.D.	343	1.07	1.00	1.04	0.99	0.6	1.00	1058.	34.6	1.6	3614.2	100.4	344.8	234.0	0.0	0.0
N.D.	344	1.08	1.00	1.04	1.00	1.2	1.00	1055.	33.9	3.1	1576.4	78.6	2884.4	134.8	0.0	0.0
N.D.	345	1.09	1.00	1.03	0.99	0.1	1.00	1077.	36.3	67.6	0.0	60.2	0.0	201.8	0.0	0.0
N.D.	346	1.08	1.00	1.04	0.99	0.2	1.00	1111.	35.4	20.9	1337.0	38.6	0.0	248.5	0.0	0.0
N.D.	347	1.07	1.00	1.03	0.99	3.4	1.00	1000.	63.3	3.7	1829.8	42.4	3597.5	79.7	0.0	0.0
N.D.	348	1.09	1.00	1.04	0.99	2.3	1.00	1000.	63.9	3.2	821.9	35.5	4141.1	131.8	0.0	0.0
N.D.	349	1.08	1.00	1.03	0.99	2.9	1.00	1011.	65.6	25.3	476.2	26.3	7271.8	388.4	0.0	0.0
N.D.	351	1.08	1.00	1.03	0.99	2.4	1.00	1044.	61.1	64.4	578.9	20.8	5572.0	204.2	0.0	0.0
N.D.	352	1.08	1.00	1.03	0.98	1.3	1.00	1033.	35.1	83.7	318.9	15.9	3667.3	179.0	0.0	0.0
N.D.	353	1.08	1.00	1.03	0.99	1.5	1.00	1061.	34.8	41.9	1336.0	27.1	3168.3	80.5	0.0	0.0
N.D.	354	1.08	1.00	1.03	0.99	1.7	1.00	1055.	34.3	32.9	222.4	26.8	4768.6	223.6	0.0	0.0
WYO.	235	0.99	0.92	1.00	0.99	-4.3	0.96	1077.	32.7	5.8	9125.8	702.3	3192.2	74.2	0.0	0.0
WYO.	236	1.00	0.99	1.00	1.00	-13.0	1.00	1055.	33.1	4.3	6357.8	668.8	3082.8	71.2	0.0	0.0
WYO.	237	1.00	1.00	1.00	1.00	-9.3	1.00	1055.	32.2	3.1	7179.5	1028.5	3075.3	71.1	0.0	0.0
WYO.	239	0.98	1.00	0.99	1.00	-1.2	0.92	1066.	33.8	10.0	13358.0	1627.7	1229.7	29.6	0.0	0.0
WYO.	290	0.97	0.00	0.98	1.00	-1.4	0.88	1075.	33.1	11.1	1387.7	1405.1	2709.0	60.7	0.0	0.0
WYO.	291	0.99	0.91	1.00	0.99	47.5	0.97	1055.	60.4	16.4	3590.5	681.2	2212.0	82.6	0.0	0.0
WYO.	292	1.01	1.00	1.01	1.01	7.3	1.00	1055.	56.0	14.2	2841.5	410.1	3167.5	138.4	0.0	0.0
WYO.	293	1.04	1.00	1.02	0.99	9.7	1.00	1055.	60.2	11.7	1836.7	276.7	3114.5	129.9	0.0	0.0
WYO.	294	1.02	1.11	1.01	1.01	4.4	1.05	1055.	57.6	8.1	2228.0	297.8	891.7	45.0	0.0	0.0
WYO.	295	1.02	1.16	1.01	1.02	2.1	1.07	1075.	59.5	11.2	851.5	156.5	1420.6	70.5	0.0	0.0
WYO.	296	1.00	1.00	1.00	1.00	13.9	1.00	1061.	58.9	9.4	9621.9	897.9	3238.6	53.1	0.0	0.0
WYO.	297	1.00	1.01	1.00	1.00	10.3	1.01	1066.	60.5	11.3	3206.3	381.2	2871.7	56.2	0.0	0.0
WYO.	298	1.02	1.13	1.01	1.01	19.1	1.05	1077.	61.4	13.7	3115.0	157.6	3069.4	103.2	0.0	0.0
WYO.	299	1.01	1.15	1.01	1.02	3.3	1.05	1100.	62.1	12.2	247.9	89.0	2972.2	118.3	0.0	0.0
WYO.	300	1.06	1.00	1.03	1.00	6.7	1.00	1122.	66.0	110.5	80.4	35.3	1681.2	101.9	0.0	0.0
WYO.	301	0.92	1.00	1.00	0.99	-1.5	0.73	1044.	32.4	4.5	20048.7	462.3	1915.5	44.7	0.0	0.0
WYO.	302	1.04	1.00	1.02	1.00	8.6	1.00	1027.	31.3	3.7	14895.5	357.3	1395.9	16.7	0.0	0.0
WYO.	303	1.07	1.00	1.04	0.99	136.8	1.00	1022.	31.8	3.0	7893.8	145.4	5651.7	96.4	0.0	0.0
WYO.	304	1.04	1.00	1.02	1.00	5.5	1.00	1039.	31.0	14.1	4763.6	241.0	1013.7	75.2	0.0	0.0
WYO.	305	0.98	1.00	0.99	1.00	0.0	0.92	1055.	31.9	20.5	10706.3	679.2	225250.4	142.6	0.0	0.0
WYO.	306	1.01	1.08	1.00	1.00	-4.7	1.03	1000.	61.2	188.3	3020.5	1112.3	2278.4	99.7	0.0	0.0
WYO.	308	1.05	1.00	1.02	1.00	10.4	1.00	1019.	62.5	295.1	1675.6	214.7	2486.5	138.0	0.0	0.0
WYO.	309	1.08	1.00	1.05	0.99	-5.4	1.00	1005.	59.7	773.2	4356.8	717.0	2202.2	94.6	0.0	0.0
WYO.	310	1.01	1.00	1.01	1.00	6.7	1.00	1000.	58.2	918.2	3163.7	765.6	2803.6	152.3	0.0	0.0
WYO.	312	1.02	1.00	1.01	1.00	11.2	1.07	1011.	34.1	60.3	6933.0	834.0	2305.6	81.9	0.0	0.0
WYO.	313	1.05	1.00	1.03	0.99	5.2	1.00	1022.	35.5	41.8	1812.7	460.1	2742.4	135.5	0.0	0.0
WYO.	314	1.05	1.00	1.02	1.00	5.1	1.00	1052.	32.7	60.5	4843.7	330.7	2766.5	132.1	0.0	0.0
WYO.	315	1.04	1.00	1.02	1.00	6.7	1.00	1055.	34.4	2.5	4179.8	334.0	2602.9	120.8	0.0	0.0
WYO.	316	1.03	1.00	1.01	1.00	6.2	1.06	1055.	35.2	5.1	4923.0	423.7	2851.3	122.5	0.0	0.0
WYO.	317	1.04	1.00	1.02	1.00	2.9	1.00	1061.	35.4	21.2	4895.8	530.5	2256.6	152.5	0.0	0.0
WYO.	318	1.01	1.07	1.00	1.00	17.4	1.03	1000.	60.0	20.6	7711.1	965.9	2073.0	70.7	0.0	0.0
WYO.	319	1.04	1.00	1.02	1.00	13.4	1.00	1000.	61.8	13.3	6327.7	675.6	2955.3	115.6	0.0	0.0
WYO.	320	1.04	1.00	1.02	0.99	3.6	1.00	1000.	60.7	21.6	3208.0	303.5	3386.1	158.5	0.0	0.0
WYO.	322	1.01	1.05	1.00	1.00	8.7	1.02	1000.	60.4	41.3	9504.9	1569.6	2948.3	104.9	0.0	0.0
WYO.	323	1.07	1.00	1.03	0.99	7.9	1.00	1000.	58.5	17.5	4106.3	473.7	2811.1	153.3	0.0	0.0
WYO.	325	1.02	1.00	1.01	1.00	5.3	1.08	1022.	31.9	1.0	11751.8	783.2	3118.8	121.7	0.0	0.0
WYO.	326	1.04	1.00	1.02	1.00	5.1	1.00	1022.	31.8	2.5	12531.5	1016.8	3073.8	111.6	0.0	0.0
WYO.	327	1.06	1.00	1.03	0.99	4.9	1.00	1027.	31.7	1.8	12207.9	1030.7	3066.2	121.6	0.0	0.0
ILL.	362	1.06	1.00	1.04	0.99	1.7	1.00	1111.	60.9	14.8	717.7	117.2	12939.6	807.9	0.0	0.0
ILL.	363	1.07	1.00	1.04	0.99	1.4	1.00	1105.	59.2	10.8	677.1	63.2	10983.4	663.4	0.0	0.0
ILL.	364	1.07	1.00	1.05	1.00	1.3	1.00	1116.	59.5	10.0	554.2	52.9	12217.3	878.3	0.0	0.0
ILL.	365	1.07	1.00	1.05	1.00	1.3	1.00	1127.	59.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILL.	366	1.07	1.00	1.05	1.00	1.3	1.00	1127.	59.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILL.	367	0.00	0.00	0.00	0.00	0.0	0.00	1233.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILL.	368	1.09	1.00	1.07	1.00	2.5	1.00	1247.	90.0	17.9	355.6	41.0	15785.7	1229.3	0.0	0.0
ILL.	369	1.05	1.00	1.03	1.00	2.4	1.00	1244.	87.8	13.1	428.4	44.6	17257.3	1281.0	0.0	0.0
ILL.	370	1.06	1.00	1.03	1.00	2.5	1.00	1222.	92.0	16.5	601.0	182.2	8012.1	619.8	0.0	0.0
ILL.	371	1.07	1.00	1.04	1.00	1.6	1.00	1323.	85.6	32.1	730.5	667.1	7812.2	541.5	0.0	0.0
ILL.	372	1.03	1.23	1.02	1.02	1.3	1.10	1155.	82.8	20.5	340.3	69.8	11422.4	966.8	0.0	0.0
ILL.	373	1.06	1.00	1.04	1.00	1.8	1.00	1133.	59.1	22.9	411.9	58.9	11719.3	1080.7	0.0	0.0
ILL.	374	1.07	1.00	1.05	1.00	1.5	1.00	1111.	61.2	9.3	303.0	27.6	10072.1	958.6	0.0	0.0
ILL.	375	1.07	1.00	1.05	1.00	1.6	1.00	1094.	62.0	9.5	273.0	23.1	10143.5	931.0	0.0	0.0
ILL.	376	1.09	1.00	1.06	0.99	1.4	1.00	1094.	62.9	48.5	173.9	38.5	9521.9	942.3	0.0	

APPENDIX C

SUMMARY OF INJECTOR TESTS, PARAMETRIC VARIATION AND MAPPING TESTS

TEST NO.	TABLE C1 OPTIMIZATION AND MAPPING OUTPUT OF MEASURED VALUES										CHAR ANALYSIS (WEIGHT %)										C O D E
	FLOWRATES, (KG HR)	PRIMARY		SECONDARY		N2O		N2		PURGE N2		NORMALIZED WATER-FREE GAS ANALYSIS, (MOLE PERCENT)		H2		O2		N2		C	
	COAL	AP	O2	H2O	N2	PURGE N2	AR	CO	CO2	CH4	H2	O2	N2	C	H	O	N	S	ASH		
86	33.39	1.60	22.69	4.60	0.00	0.92	3.36	10.06	48.60	2.98	15.37	3.22	3.92	83.16	1.18	0.25	1.01	0.63	14.38	A	
87	28.62	1.63	27.45	9.50	0.00	0.92	3.42	28.16	48.41	0.66	14.49	1.49	3.17	70.94	0.52	0.00	0.74	0.88	24.26	A	
88	30.13	2.65	24.48	5.00	0.00	0.92	3.57	37.94	38.50	0.36	17.94	0.32	3.39	72.21	0.49	0.00	0.74	1.11	25.43	A	
89	30.13	2.65	27.71	9.50	0.00	0.92	3.78	42.20	28.01	0.83	20.59	0.96	2.61	76.22	0.45	-0.01	0.85	0.84	21.65	A	
124	39.20	1.17	28.12	0.00	0.00	0.46	2.92	32.74	38.26	3.92	18.92	1.91	1.52	78.24	2.36	2.25	1.22	0.92	17.01	A	
125	31.90	1.26	28.12	9.50	0.00	0.46	2.59	21.97	39.07	0.65	13.01	1.14	2.07	71.27	1.38	-0.23	0.98	0.54	25.96	A	
126	27.90	1.34	33.69	5.50	1.40	0.48	3.63	23.01	54.63	0.23	10.12	2.32	5.55	71.07	0.92	-0.10	1.07	0.60	26.99	A	
127	32.70	1.42	22.96	5.20	1.40	0.48	4.06	35.28	33.48	1.45	17.46	2.18	5.91	74.07	0.78	0.10	0.97	0.48	23.28	A	
128	40.10	1.45	23.56	0.00	1.40	0.66	4.02	41.22	22.44	1.18	23.69	0.34	5.10	83.01	0.79	-0.14	1.07	0.58	14.87	A	
129	31.90	2.03	33.26	0.00	1.40	0.66	2.56	38.46	36.83	0.72	16.11	0.00	5.13	71.37	1.61	3.10	0.97	0.62	22.13	A	
130	32.80	2.03	23.30	10.00	1.40	0.66	4.36	46.46	19.44	1.31	22.74	0.94	4.80	75.27	1.00	2.09	0.95	0.64	18.45	A	
134	32.20	2.71	28.49	5.00	1.40	0.66	3.47	48.64	19.48	0.70	22.55	1.10	3.96	73.49	1.10	1.07	0.00	0.78	22.56	A	
135	27.90	1.67	28.49	0.00	1.40	0.66	3.82	38.67	33.48	0.10	16.32	1.86	5.74	78.78	1.17	-0.25	0.93	0.56	19.18	A	
137	33.30	1.50	28.57	0.00	0.00	0.30	3.55	37.96	35.62	1.77	18.34	0.94	1.33	72.46	1.03	0.55	1.04	0.59	19.43	A	
138	39.60	3.03	27.97	0.00	0.00	1.01	5.77	46.50	19.31	2.79	23.77	0.00	1.86	79.74	0.32	-0.20	0.89	0.66	19.19	A	
139	32.40	3.12	28.48	9.50	0.00	1.01	5.34	48.80	19.19	1.15	23.41	0.00	2.22	69.80	0.21	3.52	0.84	1.20	24.43	A	
140	33.40	3.18	27.72	9.50	0.00	1.01	4.71	46.52	21.31	2.26	23.12	0.00	2.08	76.60	0.86	4.42	0.92	0.64	16.56	A	
141	35.00	3.44	33.16	4.90	0.00	1.01	3.42	46.59	20.79	0.42	25.65	1.17	1.95	76.98	0.84	-1.39	1.05	0.56	19.18	A	
142	31.20	3.51	22.69	4.90	0.00	1.01	5.21	50.03	13.62	1.54	26.48	0.96	3.16	76.49	0.50	3.15	0.86	0.77	18.03	A	
143	33.10	2.66	32.99	10.20	0.00	0.75	3.62	40.68	33.13	0.22	20.38	0.00	1.97	74.48	0.35	0.16	0.76	0.65	23.60	A	
144	32.60	4.73	27.97	0.00	0.00	0.75	2.71	44.25	28.29	0.33	21.32	0.72	1.89	75.07	0.41	0.08	0.81	0.65	22.98	A	
145	32.60	3.03	27.97	9.50	0.00	0.75	3.45	49.96	39.58	0.80	20.46	0.00	2.70	79.71	2.38	1.60	0.76	0.91	24.53	A	
146	36.50	3.37	23.29	0.00	0.00	0.75	5.10	46.80	17.46	1.94	23.54	1.07	1.79	76.43	0.58	1.99	1.05	0.56	19.09	A	
147	34.32	3.63	27.73	0.00	0.00	0.92	5.54	47.22	23.85	0.62	20.03	0.86	1.86	75.69	0.35	-0.03	0.63	0.94	22.42	B	
148	34.32	3.56	27.45	0.00	0.00	0.92	5.97	48.97	22.82	0.15	18.00	0.64	3.46	69.41	0.22	-1.51	0.53	0.92	31.38	B	
149	34.32	3.56	27.45	0.00	0.00	0.92	5.97	48.97	22.82	0.15	18.00	0.64	3.46	69.41	0.22	-1.51	0.53	0.92	31.38	B	
150	33.44	3.64	27.90	0.00	0.00	0.92	5.56	50.96	19.58	0.88	14.51	2.35	5.11	69.60	0.21	-2.32	0.67	1.00	30.84	B	
151	29.92	3.60	25.07	0.00	0.00	0.92	5.88	53.76	18.46	0.33	21.58	0.00	1.98	75.33	0.25	0.12	0.80	0.72	23.76	B	
152	33.44	3.63	28.07	0.00	0.00	0.92	4.92	50.71	18.63	1.12	22.22	0.07	2.73	77.75	0.59	1.71	1.06	0.69	18.20	B	
153	33.44	3.64	28.11	0.00	0.00	0.92	4.63	48.36	12.38	0.67	17.90	4.75	15.71	71.95	0.41	-0.35	0.67	0.80	26.52	B	
154	33.44	3.64	28.11	0.00	0.00	0.92	4.63	48.36	12.38	0.67	17.90	4.75	15.71	71.95	0.41	-0.35	0.67	0.80	26.52	B	
155	33.00	3.65	27.44	0.00	0.00	0.75	3.98	0.37	39.50	0.00	0.00	59.34	3.93	13.75	0.11	7.54	0.17	1.19	78.24	B	
156	33.00	3.63	28.07	0.00	0.00	0.75	3.27	1.09	45.93	0.00	0.00	45.83	3.83	14.28	0.11	11.63	0.31	0.72	62.88	B	
157	34.60	3.63	28.07	0.00	0.00	0.75	3.66	27.32	32.86	1.36	9.28	1.11	4.02	79.91	2.04	5.81	1.16	0.48	10.60	B	
158	31.10	3.67	28.16	0.00	0.00	0.75	8.95	10.52	31.63	2.20	13.63	6.12	6.96	77.78	2.12	6.46	1.36	0.57	13.73	B	
159	36.00	3.26	28.15	0.00	0.00	0.83	1.66	0.00	30.97	0.00	0.00	61.64	6.96	69.92	2.04	3.72	1.21	0.42	24.69	B	
160	36.00	3.26	28.15	0.00	0.00	0.83	1.66	0.00	30.97	0.00	0.00	61.64	6.96	69.92	2.04	3.72	1.21	0.42	24.69	B	
161	11.40	1.10	28.04	0.00	0.00	0.83	2.46	0.00	22.42	0.00	0.00	70.38	4.24	68.40	1.54	5.55	1.54	0.29	22.68	B	
162	39.40	2.21	28.15	0.00	0.00	0.83	1.94	0.00	30.97	0.00	0.00	63.11	3.79	60.88	1.47	7.75	1.47	0.57	11.19	B	
163	11.10	1.23	28.15	0.00	0.00	0.75	2.60	0.00	41.77	0.00	0.00	52.99	2.55	65.34	0.81	0.17	0.89	0.83	31.96	B	
164	32.20	1.23	28.15	0.00	0.00	0.75	2.60	0.00	41.77	0.00	0.00	52.99	2.55	65.34	0.81	0.17	0.89	0.83	31.96	B	
165	32.20	1.23	28.15	0.00	0.00	0.75	2.60	0.00	41.77	0.00	0.00	52.99	2.55	65.34	0.81	0.17	0.89	0.83	31.96	B	
166	27.90	1.35	27.97	0.00	0.00	0.75	6.41	5.86	48.74	0.00	1.59	34.19	3.92	66.45	0.18	-0.05	0.90	0.35	45.49	B	
167	27.90	1.35	27.99	0.00	0.00	0.75	6.41	5.86	48.74	0.00	1.59	34.19	3.92	66.45	0.18	-0.05	0.90	0.35	45.49	B	
168	33.10	1.35	27.99	0.00	0.00	0.75	6.41	5.86	48.74	0.00	1.59	34.19	3.92	66.45	0.18	-0.05	0.90	0.35	45.49	B	
169	33.10	1.35	27.99	0.00	0.00	0.75	6.41	5.86	48.74	0.00	1.59	34.19	3.92	66.45	0.18	-0.05	0.90	0.35	45.49	B	
171	37.00	1.35	27.99	0.00	0.00	0.75	6.41	5.86	48.74	0.00	1.59	34.19	3.92	66.45	0.18	-0.05	0.90	0.35	45.49	B	
172	37.00	1.23	22.95	5.00	0.00	0.75	2.15	45.17	18.31	1.74	29.04	0.81	2.23	80.54	1.88	3.32	1.17	0.72	12.37	C	
173	37.00	1.23	22.95	5.00	0.00	0.75	2.15	45.17	18.31	1.74	29.04	0.81	2.23	80.54	1.88	3.32	1.17	0.72	12.37	C	
174	37.00	1.23	22.95	5.00	0.00	0.75	2.15	45.17	18.31	1.74	29.04	0.81	2.23	80.54	1.88	3.32	1.17	0.72	12.37	C	
175	32.50	1.23	22.95	5.00	0.00	0.81	3.67	51.6													

TEST NO.	ELEMENTAL CLOSURES OBSERVED - PREDICTED (MOL/MOL)										TABLE C1 OPTIMIZATION AND MAPPING OUTPUT OF COMPUTED VALUES										ENERGY BALANCE (OUT/IN)				VELOCITY (M/SEC)		MOMENTUM (PRI-SEC)		C O D E
	C	H	O	N	S	A	C	H	O	N	C	H	O	N	S	A	TOT	SENSIBLE GAS	INTERNAL GAS	CHAR LOST	PRI.	SEC.	PRI-SEC	DF					
86	0.98	0.94	0.99	0.88	0.67	0.39	1.01	0.97	1.00	1.00	0.89	0.86	0.99	0.09	0.02	0.16	0.54	0.19	14.3	15.6	1.48	-0.01	A						
87	0.93	0.93	0.99	0.83	1.09	0.37	1.03	0.34	0.96	1.00	1.33	1.03	0.93	0.13	0.02	0.20	0.40	0.26	19.3	19.3	0.74	-0.06	A						
88	1.00	1.00	1.00	1.00	1.97	0.61	1.04	0.34	0.96	1.00	1.60	0.46	0.90	0.10	0.02	0.25	0.47	0.16	19.7	19.7	1.32	-0.08	A						
89	0.93	0.93	0.99	0.80	1.21	0.39	1.02	0.37	1.00	1.00	1.11	0.90	1.00	0.13	0.01	0.33	0.30	0.24	19.3	19.3	1.92	0.02	A						
125	0.93	0.89	0.99	0.72	2.92	0.34	1.02	0.33	0.96	1.00	1.43	1.51	0.98	0.10	0.03	0.25	0.48	0.15	11.1	12.3	1.02	0.00	A						
126	0.98	0.91	0.99	0.89	0.68	0.38	1.03	0.88	0.96	1.00	0.86	1.44	0.96	0.21	0.02	0.16	0.36	0.35	12.0	25.4	0.42	-0.03	A						
127	0.98	0.91	0.99	0.90	1.46	0.90	1.04	0.76	0.92	1.00	1.36	1.41	0.39	0.15	0.03	0.24	0.54	0.04	13.5	18.3	0.97	-0.02	A						
128	0.93	0.92	0.99	0.91	1.52	0.91	0.99	1.04	0.97	1.00	1.26	1.41	1.01	0.12	0.03	0.27	0.47	0.11	4.3	3.4	1.98	0.03	A						
129	1.00	1.00	1.00	1.00	1.49	0.34	1.04	1.04	0.98	1.00	1.34	0.82	0.99	0.17	0.02	0.29	0.32	0.20	6.1	4.2	2.01	0.00	A						
130	0.93	0.93	0.99	0.90	1.73	0.91	1.02	0.96	0.97	1.00	1.40	1.35	1.00	0.20	0.02	0.34	0.38	0.06	6.1	7.9	1.23	0.01	A						
134	0.93	0.90	0.99	0.86	2.52	0.38	1.02	0.99	0.99	1.00	1.86	1.01	1.02	0.10	0.02	0.43	0.24	0.10	15.8	13.0	1.83	0.05	A						
135	0.93	0.89	0.99	0.90	0.88	0.90	1.01	1.05	0.99	1.00	0.97	1.29	1.03	0.17	0.02	0.27	0.31	0.34	15.8	13.0	1.83	0.05	A						
137	0.97	0.86	0.99	0.54	9.61	0.82	1.02	0.38	0.95	1.00	5.74	1.35	0.97	0.12	0.03	0.27	0.38	0.20	14.3	12.5	1.62	-0.01	A						
138	0.93	0.90	0.99	0.30	2.16	0.91	1.02	0.98	0.94	1.00	1.75	1.47	1.00	0.13	0.02	0.38	0.18	0.11	5.8	2.5	6.89	0.02	A						
139	0.98	0.92	0.99	0.77	4.80	0.91	1.03	0.95	0.96	1.00	2.12	1.33	1.00	0.20	0.02	0.44	0.24	0.10	5.9	5.5	2.42	0.02	A						
140	0.98	0.93	0.99	0.81	2.49	0.91	0.99	1.11	1.01	1.00	1.83	1.07	0.98	0.20	0.02	0.43	0.24	0.10	5.9	5.5	2.42	0.02	A						
141	1.00	1.00	1.00	1.00	2.38	0.62	1.02	1.18	1.00	1.00	2.03	0.85	1.05	0.19	0.02	0.41	0.24	0.13	6.2	4.7	3.19	0.07	A						
142	0.98	0.92	0.99	0.80	1.64	0.92	1.01	1.06	0.99	1.00	2.14	1.05	1.04	0.18	0.02	0.43	0.28	0.08	6.3	3.7	6.40	0.06	A						
143	0.93	0.92	0.99	0.74	2.32	0.87	1.03	0.97	0.99	1.00	1.89	0.99	1.00	0.21	0.02	0.32	0.26	0.18	7.3	9.0	1.44	0.02	A						
144	1.00	1.00	1.00	1.00	2.49	0.51	1.01	1.07	1.00	1.00	2.15	1.07	1.00	0.23	0.02	0.36	0.27	0.13	7.2	8.4	1.51	0.02	A						
145	0.93	0.90	0.99	0.74	2.91	0.90	1.03	0.95	0.97	1.00	2.15	0.99	0.96	0.13	0.03	0.36	0.44	0.04	9.7	3.1	12.10	-0.02	A						
146	0.98	0.83	0.99	0.77	5.12	0.91	1.03	0.85	0.96	1.00	2.15	0.99	0.96	0.13	0.03	0.36	0.44	0.04	9.7	3.1	12.10	-0.02	A						
147	0.93	0.87	0.99	0.76	1.04	0.92	-	-	-	-	-	-	-	-	-	-	-	-	6.7	2.4	10.10	-	B						
148	0.98	0.86	0.99	0.84	2.18	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.4	9.75	-	B						
149	0.98	0.86	0.99	0.84	2.18	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.4	10.17	-	B						
150	0.93	0.86	0.99	0.83	2.42	0.92	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.4	10.03	-	B						
151	0.93	0.88	0.99	0.76	1.54	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.8	2.4	9.87	-	B						
152	0.93	0.90	0.99	0.83	1.49	0.91	-	-	-	-	-	-	-	-	-	-	-	-	6.5	2.3	9.84	-	B						
153	0.93	0.84	0.99	0.96	3.49	0.92	-	-	-	-	-	-	-	-	-	-	-	-	6.8	2.4	9.88	-	B						
154	0.93	0.78	1.00	0.93	2.89	0.94	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.3	10.08	-	B						
155	0.93	0.79	1.00	0.89	0.00	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.3	10.24	-	B						
156	0.98	0.79	1.00	0.90	0.00	0.92	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.3	9.87	-	B						
157	1.00	1.00	1.00	1.00	0.36	1.00	-	-	-	-	-	-	-	-	-	-	-	-	6.7	2.4	9.84	-	B						
158	0.99	0.92	0.99	0.94	1.20	0.97	-	-	-	-	-	-	-	-	-	-	-	-	6.7	2.4	9.98	-	B						
159	0.98	0.91	1.00	0.97	0.00	0.91	-	-	-	-	-	-	-	-	-	-	-	-	5.9	2.4	7.81	-	B						
160	0.98	0.82	1.00	0.89	0.00	0.92	-	-	-	-	-	-	-	-	-	-	-	-	6.1	2.4	7.88	-	B						
161	0.93	0.79	1.00	0.94	0.00	0.95	-	-	-	-	-	-	-	-	-	-	-	-	6.3	2.4	8.13	-	B						
162	0.93	0.81	1.00	0.94	0.01	0.91	-	-	-	-	-	-	-	-	-	-	-	-	5.8	2.3	7.63	-	B						
163	0.98	0.83	1.00	0.88	0.88	0.91	-	-	-	-	-	-	-	-	-	-	-	-	6.0	2.4	8.03	-	B						
164	0.98	0.80	1.00	0.97	0.01	0.91	-	-	-	-	-	-	-	-	-	-	-	-	6.1	2.4	8.16	-	B						
165	0.93	0.75	1.00	0.86	0.86	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.1	2.4	8.16	-	B						
166	0.93	0.86	1.00	0.88	0.05	0.94	-	-	-	-	-	-	-	-	-	-	-	-	6.1	2.4	8.16	-	B						
167	0.99	0.95	1.00	0.99	0.49	0.99	-	-	-	-	-	-	-	-	-	-	-	-	6.1	2.3	8.87	-	B						
168	1.00	1.02	1.00	1.01	0.01	1.01	-	-	-	-	-	-	-	-	-	-	-	-	6.6	2.5	8.67	-	B						
169	0.93	0.75	1.00	0.93	0.93	0.93	-	-	-	-	-	-	-	-	-	-	-	-	6.2	2.4	8.67	-	B						
170	0.93	0.77	1.00	0.97	2.10	0.36	0.92	1.24	1.07	1.00	1.41	0.81	1.15	0.10	0.01	0.28	0.36	0.23	31.8	23.2	1.80	0.14	C						
171	0.93	0.75	1.00	0.93	1.50	0.34	0.95	1.16	1.05	1.00	1.18	1.02	1.13	0.11	0.01	0.36	0.26	0.26	27.6	23.2	1.80	0.14	C						
172	0.99	0.95	0.99	0.83	1.50	0.34	0.91	1.27	1.08	1.00	1.01	1.03	1.11	0.10	0.01	0.28	0.35	0.26	31.8	17.4	5.96	0.13	C						
173	0.99	0.96	1.00	0.87	2.02	0.39	0.99	1.12	1.02	1.00	0.97	1.21	1.07	0.11	0.01	0.42	0.21	0.26	31.8	22.8	3.34	0.09	C						
174	0.98	0.91	0.99	0.75	1.05	0.80	1.03	0.92	0.93	0.99	1.51	1.74	0.98	0.08	0.01	0.40	0.38	0.13	11.1	3.1	13.71	0.00	C						
175	0.98	0.89	0.99	0.81	1.99	0.90	1.04	0.97	0.98	1.00	1.21	1.23	1.04	0.11	0.01	0.45	0.19	0.21	12.9	7.1	4.15	-0.02	C						
176	0.98	0.92	0.99	0.77	1.27	0.31	1.04	0.39	0.96	1.00	1.50	0.92	0.95	0.13	0.02	0.40	0.40	0.06	11.1	3.1	13.71	0.00	C						
177	0.98	0.94	0.99	0.83	1.56	0.37	1.02	1.07	0.99	1.00	1.36	1.24	1.05	0.13	0.01	0.50	0.19	0.18	13.3	6.6	7.87	0.07	C						
178	0.98	0.91	0.99	0.78	1.81	0.34	1.03	0.90	0.97	1.00	1.75	1.08	0.98																

APPENDIX D
GASIFICATION TEST AND ANALYSIS PROCEDURES

GASIFICATION TEST AND ANALYSIS PROCEDURES

The procedures used to operate the gasifier at atmospheric pressure have been detailed by Skinner (1980), Highsmith (1982), Soelberg (1983), Brown (1985), and at elevated pressure by Anderson (1983). Similarly, analysis procedures have been discussed in detail by Price (1980), Burkinshaw (1981), Highsmith (1982) and Nichols (1985). Some modifications in the analysis and operating procedure were implemented in this study. A brief summary of these testing procedures follows. Additional procedural details can be found in Sowa (1987) and Nichols (1987).

Test Procedures

Because operation at elevated pressure was very similar to the operation at atmospheric pressure both cases will be described at the same time.

A typical gasification run required eight to twelve hours with a minimum of three operators. Different phases of operation included instrument calibration and startup, reactor ignition and preheat, stabilization of coal flame, sampling, reactor cool-down, and sample analysis.

Instrument Calibration and Startup. Instruments that needed calibration were the gas chromatographs, ion-selective electrodes, and online instruments. Equipment that required warmup were the gas chromatographs, signal amplifiers, online instruments and steam boiler. The thermal conductivity detector (TCD) gas chromatograph was turned on at least 4 hours before the gasification flame sampling started. Calibrations were started one hour after turning on the chromatograph detection cells. All online instruments, steam boiler (if used), and signal amplifiers were turned on two hours before gasification flame sampling and calibrated at most one-half hour before sampling. Power to the facility, instruments, and building fans was switched on. All open loop control power supply units were turned on. The high pressure air to the facility was also opened and the regulator set at 550 psig. All control valves and ball valves were then checked to verify proper position (open or closed) for the beginning of the test. The gas manifolds were opened and facility regulators set for proper operating pressures. The coal feeder was pressure-tested to verify that no leaks existed. Deionized water for the probe was then turned on to protect the sample probe during ignition and preheat. All facility alarms (CO level, injector temperature) were checked for good operation. The load cell that measures coal feed was calibrated. The facility was then ready for ignition and preheating.

Ignition and Preheat. For ignition and preheat, the natural gas manifold was opened and regulator set at 375 psig. The operational warning lights were turned on. Window purge gas was then started at a low flow rate. Natural gas and oxygen or air were started through the injector primary and secondary ports respectively at very low flow rates. Ignitor air was turned on and hydrogen was turned on. The ignitor toggle switch was pushed to generate a spark to ignite the hydrogen-ignitor air mixture. The hydrogen flame propagated down the ignitor tube to the natural gas-air (or oxygen) stream where it ignited the natural gas-air (or oxygen) mixture. Stable methane-air (or oxygen) ignition did not occur during every ignition attempt. Between ignition attempts, the hydrogen stream was turned off. Upon successful

ignition, the hydrogen and ignitor air were turned off and the natural gas and air (or oxygen) flowrates were increased to predetermined levels. The temperature recorder was turned on. The probe water flow rate was set to an adequate level to protect the probe and the window purge flow rate was increased. The reactor was preheated until the reactor section 18 cm below the injector reached 920 K. The preheat usually took 1.5 to 2 hours when preheating with air and 45 minutes to an hour when preheating with oxygen. All preheating was done at atmospheric pressure.

Coal Flame Stabilization. When the preheat was finished, the coal feeder was pressurized to 2 psig pressure and the coal feed valve was open, the coal feed auger turned on and brought to the desired rpm. When the coal flame was stable, the natural gas was turned off. Depending on the test, either primary or secondary oxygen was turned on and any other air or oxygen used during preheat was turned off. The flame was allowed again to stabilize before any further adjustments were made. If the test was to be conducted at elevated pressure, the quench water and deionized water pumps would be turned on and the exhaust gas and sewer pressure control bypass legs closed at this point to begin pressurization. Pressurization was accomplished by slowly closing the throttling control valves on the exhaust gas and sewer discharge lines. The argon feed rate was also increased to maintain a stable flow of coal feed to the reactor. When stable operation was achieved, the steam control valve was opened and the steam flow was stabilized.

Sampling. Sampling was started when reactor stability was evident. Samples were then taken with the water-quenched sample probe positioned at various radial locations at the preset axial location. The process of sample system purging, gas and solid/liquid sample collecting, nitrogen oxide measurement, and recording in logbooks all pertinent feedstream settings and reactor conditions required on the average five minutes per sample. No attempt was made at isokinetic sampling. After each sample was collected and logged, then the set points of the feed streams could be changed or the sample probe repositioned radially and the sampling procedure repeated. The gas and solid/liquid samples were stored for later analysis.

Shutdown. After sampling was completed, the reactor shutdown began. The coal and oxygen feed streams were turned off while at pressure and the control valves controlling reactor pressure were opened. When the reactor pressure was below 2 atm, the quench water and deionized water pumps were turned off. A natural gas-air (or oxygen) flame was used after some firings to help clean the slag from the reactor walls. In such cases, the natural gas-air (or oxygen) flame was turned on at atmospheric pressure. After 20 minutes of post-test natural gas burning, the facility was shutdown with only a slow flowrate of secondary air left on to protect the injector from overheating. The probe water and exhaust gas quench water were also left on to protect the probe and exposed metal surfaces from overheating. The pressure in the coal feeder was reduced and the facility was shutdown in the reverse order that it was started. After every thermocouple in the reactor walls registered temperatures below 580 K, the facility was completely shutdown and all feed lines drained.

While the reactor was cooling, analysis of the collected gas, liquid, and char samples was initiated. Gas samples were analyzed for the major gas species, CO, CO₂, CH₄, H₂, N₂, O₂, Ar, and He. The gas samples were also

analyzed for the minor gas species H_2S , SO_2 , COS , and CS_2 . The liquid samples were analyzed for nitrogen and sulfur species. The solid material in the liquid was filtered and dried and then analyzed for elemental C,H,N,S and ash.

Chemical Analysis Procedures

Fuel and Tracer Gas Analysis. The analytical procedures used in this study are primarily those developed by Price (1980) and Burkinshaw (1981). The analysis of the gas species (H_2 , Ar, O_2 , CO_2 , N_2 , CH_4 and CO) was performed with the use of an HP-5832A gas chromatograph equipped with a thermal conductivity detector (TCD). Helium was used as the carrier gas at a flow rate of 24 ml/min. The samples to be analyzed were injected into the sample valve directly from the sample gas collection bags. In order to obtain complete separation of these gases, a 6 ft. by 1/8 in. stainless steel Porapak Q 80/100 column and a 16 ft. by 1/8 in. stainless steel Molecular Sieve 5A 60/80 column were used in a series/by-pass configuration (Hedman, et al., 1981). A time-temperature program was used to allow argon and oxygen to be detected initially. Then, a valve was switched to allow CO_2 to elute from the Porapak Q column before it entered the molecular sieve column. This was necessary because CO_2 binds irreversibly to the molecular sieve. Following the detection of CO_2 , the valve was switched back to the series configuration to allow for the detection of the remaining gases.

The determination of He as well as a second determination of H_2 were performed on an HP-5735A gas chromatograph, also equipped with a thermal conductivity detector. The samples to be analyzed by this chromatograph were injected through a septum using a 0.5 ml syringe. Two 6 ft. by 1/8 in. stainless steel Porapak Q columns were connected in series to allow for the detection and separation of H_2 and He.

Sulfur and Nitrogen Pollutant Gas Analysis. The sulfur species in the gas phase, COS (carbonyl sulfide), H_2S (hydrogen sulfide), CS_2 (carbon disulfide) and SO_2 (sulfur dioxide) were analyzed using a flame photometric detector (FPD) in an HP-5735A chromatograph interfaced with an HP-3390A integrator. A 9 ft. by 1/8 in. Teflon Chromasil Model 310 column was used. A time-temperature program was employed such that initially a lower oven temperature (25°C) was maintained while the COS and H_2S were eluted, after which the oven temperature was raised (60°C) to elute the CS_2 and SO_2 . This method was developed by Highsmith (1982). Commercially prepared standards of H_2S , COS and SO_2 were used for calibration. A calibration standard for CS_2 was made by injecting a known volume of liquid CS_2 into a known volume of nitrogen gas. The sulfur gas analyses normally occurred within 2-4 hours from the time the samples were collected.

Measured nitrogen species from the gasifier were N_2 (molecular nitrogen), NO (nitric oxide), NH_3 (ammonia), and HCN (hydrogen cyanide). NO levels were measured with a chemiluminescent NO/ NO_x analyzer. This instrument produced ozone, which reacted with NO and emitted chemiluminescence. The output from a photomultiplier which detected this emission was linearly proportional to the NO concentration. Periodically, Drager tubes were used to determine the NH_3 and HCN gas phase concentrations. These were considered negligible in most cases.

Liquid Phase Analysis. Because the gasifier sample was contacted with the probe water and quenched, some gas dissolved in the water. For this reason, the liquid phase of the sample was analyzed for dissolved product species. Most of the gases of interest are essentially insoluble in water. Those which are appreciably soluble are the pollutant species H_2S , SO_2 , NH_3 , and HCN . Aliquots of the liquid sample were treated to preserve H_2S by adding a 50 ml aliquot of liquid sample to 50 ml of anti-oxidant buffer. The buffer maintained the mixture at a high pH (11-12) so as to keep the dissolved H_2S in the form of $\text{S}^{=}$ ion. The $\text{S}^{=}$ was then detected using an Orion model 94-16A $\text{S}^{=}$ ion specific electrode in conjunction with an Orion Model 90-01 reference electrode.

The NH_3 was preserved by adding 1 ml of 0.1 M HCl to a 100 ml aliquot of liquid sample. This lowered the pH and preserved the ammonia as NH_4^+ . The NH_4^+ ion was converted back to NH_3 just prior to analysis by addition of 1 ml of 10 M NaOH . Analysis was accomplished using an Orion Model 94-10 gas sensing electrode.

The HCN was preserved by adding 1 ml of 10 M NaOH to a 100 ml aliquot of liquid sample. This raised the pH and preserved the HCN as CN^- ion. Analysis was accomplished with an Orion Model 94-06 CN^- ion specific electrode in conjunction with the reference electrode.

The SO_2 was preserved as $\text{SO}_4^{=}$ ion. This was accomplished by adding 5 ml of 30% H_2O_2 to a 50 ml aliquot of liquid sample. The $\text{SO}_4^{=}$ ion concentration was then determined using a high pressure liquid chromatograph (ion exchange column). The measured $\text{S}^{=}$ ion concentration was subtracted from the measured $\text{SO}_4^{=}$ ion concentration, and the remaining $\text{SO}_4^{=}$ was assumed to have originated from SO_2 . These liquid concentrations were converted to gas phase concentrations from a knowledge of the relative flow rates of liquid and gas from the probe.

Solids Analysis. The char (solid) portion of each sample as well as coal samples were analyzed for the relative amounts of carbon, hydrogen, nitrogen, sulfur, and ash which they contained. Carbon, hydrogen and nitrogen were determined using a Leco Model CHN 800 elemental analyzer. This instrument required only 5-10 mg of solid sample per analysis. Analysis time was 3-4 minutes per sample. The sample was combusted with high-purity oxygen. The resulting gas passed through an IR cell for detection of CO_2 and through a second IR cell for detection of H_2O . An aliquot of the gas was passed through a catalyst bed at high temperature which converted nitrogen oxides to N_2 , and the N_2 was subsequently detected in a thermal conductivity cell. The relative amounts of CO_2 , H_2O , and N_2 in the combustion gas were then used to provide a measure of the weight percent of C, H, and N in the solid.

Sulfur was determined using a Leco Model 634-800 sulfur analyzer. A sample size of 50 mg was required. The sample was combusted with oxygen. The resulting gas was bubbled through a solution of starch indicator, potassium iodate, and hydrochloric acid. The starch indicator formed a complex with the iodate ion, which caused the solution to appear blue in color. The SO_2 from the gas destroyed the complex by reacting with the iodate in the complex, thus tending to remove the blue color. As the blue color diminished, the change in color was detected by a photomultiplier tube. More potassium iodate was automatically titrated to return the solution to the blue color. The amount

of potassium iodate titrant used was proportional to the amount of SO_2 , which was assumed to be proportional to the amount of sulfur in the solid sample.

The ash content was determined using a variation of ASTM method D 3174-82. The ASTM procedure called for 1 g of sample. The weight of char samples collected from the gasifier was often less than 1 g. The sample was heated from room temperature to 750°C over a two hour period, and then maintained at 750°C for two additional hours. The material remaining after the four hours was designated as ash.

Data Analysis Procedures

Data analysis methods were examined in great detail to improve computational accuracy, and to assure a consistent set of assumptions for all computations. This section summarizes the approach used and the basic assumptions in the data reduction methods.

Water Mole Fraction. The use of water-quenched sample probes precludes direct measurement of forced water mole fraction in the exhaust gases. Thus, it is necessary to calculate the water mole fraction through forced mass balance relationships (Mountain Fuel Resources, 1986; Brown, 1985; and Asay, 1982). This estimation procedure is subject to uncertainty when applied to a system such as the BYU gasifier where the variance associated with any property measurement can be quite large. Because of the normal experimental errors involved, a large difference in the predicted water mole fractions is generally experienced depending on the particular elemental mass balances that are being forced. Table D-1 shows an example of the expected water mole fractions found by solving four simultaneous mass balance equations, one for each of the four unknown variables. These results illustrate that the predicted water mole fraction is clearly dependent on the particular mass balance equations that are used. The range in the predicted water mole fractions was due to the accuracy of the measurements of each element and the weakness of the assumption that a single measurement can be used to represent mean properties at a given set of conditions. If all of the experimental measurements had very small variances and no random or systematic errors, then the predicted values of the water mole fraction would all be the same.

To improve the method for estimating the water mole fraction from a single combination of elements, an algorithm was developed and used throughout this study to estimate the water mole fraction. The first step in the algorithm was to set up necessary tables of elemental flow rates into the reaction chamber and measured elemental molar concentrations in the exhaust gas, measured on a dry basis. All possible elemental combinations were then used in solving simultaneous mass balance equations to approximate the water mole fraction. Each solution was checked to verify that the water mole fractions were realistic ($0 < \text{water mole fraction} < 1.0$) and that the mass balance combination used was not simply a permutation of a previously used elemental combination. Every solution that passed these checks was then tabulated and finally averaged to estimate the most likely value of the water mole fraction based upon the available input data.

TABLE D-1

PREDICTED VALUES OF THE MOLE FRACTION OF WATER IN THE EXHAUST GAS
USING DIFFERENT MASS BALANCE COMBINATIONS

The Following Data Summary is for Sample Number 187 and is Based on
Observed Values Only

Forced Mass Balances Elements Used				Predicted Values % H ₂ O
C	H	O	N	15.4
C	H	Ar	N	14.8
C	O	Ar	N	40.4
H	O	Ar	N	13.0
H	N	Ar	S	25.0

Isokinetic Sampling. Isokinetic sampling requires that the magnitude and direction of the velocity of the gas in the sampling probe match the magnitude and direction of the gas in the main stream (Work and Warner, 1981). Isokinetic sampling was attempted and found to be very difficult in past studies in turbulent, particle-laden flames at BYU using sampling probes that were similar to those used in this study (Asay, 1982). No attempt was made during this study to sample isokinetically.

To get around the problem of non-isokinetic sampling, past data analysis procedures attempted to scale local measurements by an isokinetic correction factor (Brown, 1985; and Asay, 1982). Isokinetic correction factors are important if the measurement of local mass fluxes or the determination of particle size distribution of the collected particulate is desired. No attempt was made in this study to measure local particle or gas mass fluxes or local char particle size distributions. All of the sampling that was done throughout this study was done at suction rates that were greater than the correct isokinetic suction rate. The impact of this problem has not been quantified. However, qualitatively, the greater suction rates suggest that every sample came from a greater local volume than existed in free stream flow directly above the cross-sectional area of the sampling probe tip. The particles sampled may have also been slightly biased by collecting too many of the smaller particles. It has been suggested that it is better to err on the side of oversuction than undersuction relative to isokinetic conditions (Beer, 1980).

Local Mass Balances. Local mass balances were used to determine water mole fraction and to determine the local gas mixture fraction, the coal mixture fraction, and mixture fraction of the window purge gas. A complete description of the data reduction equation, computer code and data reduction procedure is contained in Sowa (1987). A brief summary follows. Equation D-1 is the general form of the local mass balance equation.

$$w_i^{\text{local}} = n w_i^{\text{coal}} + \gamma w_i^{\text{window}} + f w_i^{\text{primary}} + (1-n-\gamma-f)w_i^{\text{secondary}} \quad (\text{D-1})$$

where: w_i^{local} $\equiv$ local gas mass fraction of element i
 w_i^{coal} $\equiv$ mass fraction of element i in raw coal
 w_i^{window} $\equiv$ mass fraction of element i in window purge stream
 w_i^{primary} $\equiv$ mass fraction of element i in primary stream
 $w_i^{\text{secondary}}$ $\equiv$ mass fraction of element i in secondary stream

$$n = \dot{m}_{i,\text{coal}}^{\text{gas}} / \dot{m}_i^{\text{total}}$$

$$\gamma = \dot{m}_{i,\text{window}}^{\text{gas}} / \dot{m}_i^{\text{total}}$$

$$f = \dot{m}_{i,\text{primary}}^{\text{gas}} / \dot{m}_i^{\text{total}}$$

The left hand side of this equation can be written in terms of the local water mole fraction resulting in Equation 2.

$$w_i^{\text{local}} = \frac{(\sum_k v_i Y_k (1-Y_{\text{H}_2\text{O}}) + v_i Y_{\text{H}_2\text{O}}) \text{MW}_k}{\text{MW}_D (1-Y_{\text{H}_2\text{O}}) + \text{MW}_{\text{H}_2\text{O}} Y_{\text{H}_2\text{O}}} \quad (\text{D-2})$$

where: i element subscript
 k species subscript
 v_i elemental stoichiometric coefficient
 Y_k species mole fraction
 $Y_{\text{H}_2\text{O}}$ mole fraction H_2O
 MW molecular weight
 MW_D dry gas molecular weight

The only unknowns are the mole fraction of water and the three progress variables, n , γ and f . Since more than four elements were followed throughout this study, the four unknowns can be determined by solving four simultaneous elemental equations. The progress variables (n , γ , and f) describe mass fractions of the local gas sample attributed to each input stream. Using this approach to determine the local water mole fractions is of great value, because the comprehensive code, PCGC-2, uses progress variables as part of its computational method (Smith and Smoot, 1985). The experimentally determined progress variables can be compared to the progress variables predicted by PCGC-2.

The local mass balance equation concept can be applied to any conserved scalar property (Smith and Smoot, 1985). The assumptions are that: 1) all eddy diffusivities for a given input stream are equal, 2) the conversion of elements in the coal occurs at the same rate, and 3) the water mole fraction is the only major species mole fraction that is unknown. The last assumption applies to the way the equation is being used and not to the equation itself. If average properties for an axial plane are desired, a local mass flux profile must still be assumed with this method. However, the strength of this method is that no local values need to be back-calculated from average properties obtained from overall mass balance equations.