PARTICULATE BEHAVIOR IN A CONTROLLED-PROFILE PULVERIZED COAL-FIRED REACTOR: A STUDY OF COUPLED TURBULENT PARTICLE DISPERSION AND THERMAL RADIATION TRANSPORT

Final Technical Progress Report

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FORWARD

This document is the final report which summarizes the technical results of a three-year study conducted for the Department of Energy (DOE) under contract number DE-FG22-91PC91308. The principal investigators for this work are Dr. Mardson Queiroz and Dr. Brent W. Webb; Dr. Clifford Smith and Dr. Phil Goldberg served as technical representatives for DOE.
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ABSTRACT

To aid in the evaluation and development of advanced coal-combustion models, comprehensive experimental data sets are needed containing information on both the condensed and gas phases. To address this need, a series of tests were initiated on a 300 kW laboratory-scale, coal-fired reactor at a single test condition using several types of instrumentation. Data collected on the reactor during the course of the test includes: gas, particle, and wall temperature profiles; radiant, total, and convective heat fluxes to the walls; particle size and velocity profiles; transmission measurements; and gas species concentrations. Solid sampling was also performed to determine carbon and total burnout. Along with the extensive experimental measurements, the particle dispersion and radiation submodels in the ACERC comprehensive 2D code were studied in detail and compared to past experimental measurements taken in the CPR. In addition to the presentation and discussion of the experimental data set, a detailed description of the measurement techniques used in collecting the data, including a discussion of the error associated with each type of measurement, is given.
NOMENCLATURE

Symbols

$a_n$ Legendre coefficients of Dirac-delta phase function approximation, dimensionless
$A$ Area, m$^2$
$b$ Two-color pyrometer calibration constant, dimensionless
$b_n$ Coefficients of Legendre series, dimensionless
$B$ Burnout, percentage
$C_1$ Planck's first constant, 37413 Wμm$^4$/cm$^2$
$C_2$ Planck's second constant, 14388 μmK
$D$ Diffusivity, m$^2$/s
$f$ Drag force, N/m$^2$
$f_f$ Fraction of forward scattering, dimensionless
$f(T_{di})$ Temperature correction factor for detector the two-color pyrometer, dimensionless
$f_v$ Soot volume fraction, dimensionless
$g$ Gravitational acceleration, m/s$^2$
$E$ Emitted energy flux, W
$I$ Intensity, W
$I_l$ Intensity, W/m$^2$srμm
$L$ Path length, m
$P_i$ $n^{th}$ Legendre polynomial, dimensionless
$q$ Heat flux, kW/m$^2$
$r$ Radial coordinate, m
$s$ Unit vector with components $\mu$, $\eta$, $\xi$, dimensionless
$S_n$ Quadrature of order $n$ in Discrete Ordinates Method
$S$ Swirl number, dimensionless
$t$ Time, sec
$T$ Temperature, K
$T'$ Temperature fluctuation from the mean defined as (T-T_m), K
$v$ Velocity, m/s
$V$ Detector voltage, V
$X$ Mass fraction, mass of species i divided by total mass
$z$ Axial coordinate, m
$\alpha$ Mass, kg
$\epsilon$ Emissivity, dimensionless
$\kappa$ Extinction or absorption coefficient, m$^{-1}$
$\lambda$ Wavelength, μm
$\Phi$ Phase function, dimensionless
$\mu_s$ Cosine of scattering angle, dimensionless
$\sigma$ Scattering coefficient, m$^{-1}$
$\tau$ Transmissivity, dimensionless

Subscripts

a Ash
b Blackbody
c Convective component
cb Carbon
cl Coal
con Convective
d Detector
d Diffusive component
gas Property of the gas
i $i^{th}$ species
j $j^{th}$ particle size
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
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<tr>
<td>L</td>
<td>Pertaining to after passing through the absorbing medium</td>
</tr>
<tr>
<td>m</td>
<td>Mean value</td>
</tr>
<tr>
<td>p</td>
<td>Probe</td>
</tr>
<tr>
<td>pc</td>
<td>Particle Cloud</td>
</tr>
<tr>
<td>rad</td>
<td>Radiative</td>
</tr>
<tr>
<td>tot</td>
<td>Total</td>
</tr>
<tr>
<td>w</td>
<td>Wall</td>
</tr>
<tr>
<td>s</td>
<td>Sample</td>
</tr>
<tr>
<td>t</td>
<td>Total</td>
</tr>
<tr>
<td>w</td>
<td>Wall</td>
</tr>
<tr>
<td>0</td>
<td>Pertaining to before passing through the absorbing medium</td>
</tr>
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<td>1</td>
<td>Pertaining to the 1.60 μm wavelength measurement of the two-color pyrometer</td>
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<tr>
<td>2</td>
<td>Pertaining to the 1.27 μm wavelength measurement of the two-color pyrometer</td>
</tr>
<tr>
<td>λ</td>
<td>Function of wavelength</td>
</tr>
</tbody>
</table>

**Superscripts**

- t: Turbulent
1. INTRODUCTION

Coal is used in large quantities for the generation of electrical power and heat for residential and industrial purposes. The process of coal combustion has proven to be very complex, involving many coupled phenomena such as turbulent fluid mechanics, particle dispersion, gas phase mixing and reaction, as well as other aspects of particulate combustion (Smoot, 1984). To analyze and improve the combustion and heat transfer, as well as to solve environmental problems involving the pollutants generated during the combustion process, advanced computer codes are needed. Models for use in predicting the operation of coal-burning facilities that are accurate and economical to use are still in the development stage. To aid in the evaluation and development of advanced coal-combustion models, comprehensive experimental data sets are needed containing information on both the condensed and gas phases. It has been noted in the literature that little data of this type are available to those working on the developed of comprehensive, pulverized-coal combustion codes (Phillips, 1989 and Truelove, 1986). Butler and Webb (1993) reviewed available data sets for pulverized-coal combustion. Their review showed that although certain data were available, complete data sets for gas and particle information at one condition were lacking. Recent research focuses on a few measurements, such as Fiveland and Latham (1993), who measured gas temperature, NO\textsubscript{X} concentration, O\textsubscript{2} profiles, and velocities. Weber et al. (1995) even used data from natural gas flames to validate their coal combustion model.

In order to fill the need for more complete data sets for pulverized-coal combustion modeling, a series of tests were performed in the laboratory-scale, Controlled Profile Reactor (CPR) at Brigham Young University (BYU). Testing was designed to obtain a full set of accurate data at a single test condition that could be used in validation of pulverized-coal combustion codes. Data reported includes: gas, particle, and wall temperature profiles; radiant, total, and convective heat fluxes to the walls; particle size and velocity profiles; transmission measurements; and gas species concentrations. Solid sampling was also performed to determine carbon and total burnout. The following section contains a description of the test facilities, sampling apparatus and procedures followed during the experiments. This is followed in section three by the presentation and discussion of the collected data. The particle dispersion and radiation submodels in
the ACERC comprehensive 2D code were also studied in detail and compared to past experimental measurements taken in the CPR. A discussion of these two models and the predictions made using them is given in section four.
2. EXPERIMENTAL PROCEDURE AND APPARATUS

Tests were performed on the Controlled-Profile Reactor (CPR) from July to September, 1993. Four shakedown tests were used as preparation for the collection of a full set of combustion measurements that could be used to verify combustion models and submodels. Care was taken during the first few tests to make the necessary adjustments that would permit uniform conditions during the two reported tests of 9/1 - 9/2, and 9/10 - 9/11. The final testing procedure and apparatus description are contained in this section.

2.1 Controlled-Profile Reactor (CPR) Operation and Description

The CPR located at Brigham Young University is a coal-burning, 300 kW, down-fired reactor with an automated feed system and extensive instrumentation to measure inlet air flow rates and wall temperatures. The reaction chamber is 80 cm in diameter and 240 cm in length, not including the tapered quarl sections on the top and bottom of the reactor (see Fig. 1). There are probe access openings located at 90° intervals around the reactor. Each large rectangular opening has two circular ports allowing probe entry at two distinct axial locations. Port numbers and axial positions, measured from the bottom of the inlet quarl, are shown in Fig. 1. Most measurements were made from the south side of the reactor, but symmetry tests were performed from the north, south and west sides. Additional description and schematics of this reactor can be found in Eatough (1991) and Butler (1992).

Coal feed rates ranging from 1 to 25 kg/h are possible with the newly modified feed system. This system was calibrated and checked frequently during the test series. Calibration was accomplished by measuring the mass of coal leaving the auger in 60 second intervals. Repeated tests at the 16 kg/hr setting showed that over a 60 second period the measured feed rate was within 2% of the set feed rate. Coal is fed from a bin by an auger-type feeder using a solid-core, single-flute auger (see Fig. 2). As the coal drops from the end of the auger, it falls onto a vibrating chute that serves two purposes: first, it smooths the pulsations as the coal leaves the auger; and second, it funnels the coal into the primary air stream by introducing it at the low pressure region of a Venturi nozzle. After entrainment, the air-coal mixture flows.
Fig. 1 - Schematic diagram of the Controlled Profile Reactor.
Fig. 2 - Schematic diagram of the new coal feeding system.
inside a tube to the primary inlet at the top of the CPR. In this manner, a steady flow of coal into the reactor is maintained.

Air flow rates into the CPR are controlled to provide fixed stoichiometry and flame stability. Compressed air is fed into the reactor through the primary and secondary lines. The primary air stream flow rate is approximately 12% of the flow rate in the secondary air stream. Flow rates are adjusted by valves and calculated from pressure measurements upstream of choked flow orifices. The pressure measurements were taken by calibrated pressure transducers, upstream of the 2.79 mm and 7.06 mm diameter orifices in the primary and secondary air flows, respectively. The discharge coefficients for the orifices were taken to be 0.95. Detailed records of mass flow rates were recorded for each test. This record consisted of mass flow rates calculated from pressure measurements taken at one minute intervals during the testing. These data indicated that fluctuations in mass flow rates were less than ±1% during the test periods.

The wall temperature acquisition system consisted of 116 thermocouples embedded in the ceramic lining of the reactor. Each thermocouple was embedded to within 2 mm of the fire side wall. Data from each thermocouple was sampled every 2 minutes using 4 multiplex boards connected in series. These boards provided ice-point calibration and computer accessibility for temperature acquisition. The signal from the thermocouples was sent to the computer where the measured voltage difference was used to calculate wall temperatures.

The CPR was preheated with natural gas before each test until the walls reached temperatures above 1300 K to provide the necessary environment to sustain combustion of the solid fuel. If the coal was fired before the walls were hot enough, steady-state, coal-fired operation could not be maintained. An emphasis was placed on keeping the reactor running in a stable manner without large changes in flow or feed conditions. Reactor stability was verified by both visual observation and experimental measurements. The coal feed rate was calibrated and found to be accurate to within ±0.25 kg/h. Data for the primary and secondary air flow rates were also carefully monitored and showed only ±1% variation during the tests. In addition to steady flow conditions, maintenance of flame symmetry in the reactor was considered essential. Before each test, the primary tube was adjusted to center the fireball in the quarl of the reactor. The flame position was visually checked between each probe exchange and adjusted if necessary. After
adjustments, both visual and experimental measurements with the suction pyrometer verified that symmetry was achieved. Representative measurements are shown in Fig. 3. Tests were performed at the ports located either at 15 or 30 cm below the quart, because this region was where the fire ball was located and where the temperature gradients were the largest. The figure shows the symmetrical nature of gas temperature measurements inside the reactor. The peaks on each side of the centerline in Fig. 3 indicate an approximate position of the flame front. The flame front was considered centered when both visual and experimental observations of the top ports showed symmetry.

2.2 Operating Conditions

The data reported were taken during two tests at the same operating conditions. During the first test (9/1/93 - 9/2/93), measurements were taken with the suction pyrometer, the two-color pyrometer, the heat flux probes, and the gas and particle sampling probe. During the second test (9/10/93 - 9/11/93), data were taken with the PCSV, the transmissometer, the heat flux probes, and the suction pyrometer. Average operating conditions during the test, along with their uncertainty are shown in Table 1. The reactor inlet flow had a swirl number of 1.4, this helped assure flame stability in the reactor. The swirl generator and number are discussed in detail in Eatough (1991). The CPR was fired with Pittsburgh #8 coal. A proximate and ultimate analysis of the coal is listed in Table 2.

2.3 Experimental Measurements and Apparatus

Testing was done to obtain profiles of particle, gas and wall temperatures. Other measurements consisted of radiative and total heat fluxes, particle size and velocity distributions, transmission measurements, gas species concentrations and particle burnout. Obtaining these data required the use of several probes. Gas temperature was measured with a suction pyrometer, particle temperature with a two-color pyrometer, and wall temperature with embedded thermocouples. A radiometer, and total heat flux probe were used to measure heat fluxes to the walls. The velocity and particle size distributions were measured with the Particle Counter Sizer Velocimeter (PCSV) probe and a transmissometer. Species concentrations and solid samples were obtained with an isokinetic sampling probe connected to a Lancom
Fig. 3 - Representative suction pyrometer symmetry measurements.
Table 1 - Operating Conditions for the CPR during Tests 1 and 2.

### AVERAGE OPERATING CONDITIONS

<table>
<thead>
<tr>
<th></th>
<th>Test 1</th>
<th>Test 2</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary Air (kg/h)</td>
<td>14.91</td>
<td>14.77</td>
<td>± 1%</td>
</tr>
<tr>
<td>Secondary Air (kg/h)</td>
<td>113.83</td>
<td>114.74</td>
<td>± 1%</td>
</tr>
<tr>
<td>Total Air (kg/h)</td>
<td>128.74</td>
<td>129.51</td>
<td>± 1%</td>
</tr>
<tr>
<td>Coal Feed Rate (kg/h)</td>
<td>16.0</td>
<td>16.0</td>
<td>± 2%</td>
</tr>
<tr>
<td>Stoichiometry</td>
<td>0.757</td>
<td>0.761</td>
<td>± 2%</td>
</tr>
</tbody>
</table>

Table 2 Analysis of the Pittsburgh #8 Coal.

### PITTSBURGH #8 COAL

<table>
<thead>
<tr>
<th>Proximate Analysis</th>
<th>Ultimate Analysis (Dry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash</td>
<td>Carbon</td>
</tr>
<tr>
<td>Volatile Matter</td>
<td>Hydrogen</td>
</tr>
<tr>
<td>Fixed Carbon</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>Moisture</td>
<td>Sulfur</td>
</tr>
<tr>
<td>HHV (KJ/kg)</td>
<td>Ash</td>
</tr>
<tr>
<td>MAF (KJ/kg)</td>
<td>Oxygen (dif)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>6.48%</td>
<td>78.71%</td>
</tr>
<tr>
<td>36.94%</td>
<td>5.15%</td>
</tr>
<tr>
<td>56.58%</td>
<td>1.56%</td>
</tr>
<tr>
<td>1.94%</td>
<td>1.55%</td>
</tr>
<tr>
<td>32618</td>
<td>6.48%</td>
</tr>
<tr>
<td>34878</td>
<td>6.55%</td>
</tr>
</tbody>
</table>
3400 gas analyzer. Each probe had to have access to the different ports of the reactor in order to provide characteristic mappings. Only one probe was used in the CPR at a time so that upstream probes would not cause flow variations affecting the downstream measurements. In order to minimize leakage into the reactor, all ports not in use were kept closed so that the reactor seal would be maintained. Taking a full set of data with all of the probes used in this study required the reactor to operate with coal at steady-state for approximately 24 hours.

In the following subsections a brief discussion of the physical characteristics of the instrumentation used is presented as well as discussions on the operation and theory behind each measurement technique. Estimated errors associated with the measurements are also presented.

2.3.1 Suction Pyrometer. The suction pyrometer probe was used to obtain gas temperatures at various axial and radial positions in the reactor. The probe consisted of an S-type thermocouple (platinum vs. platinum-10% rhodium) enclosed in a water-cooled, stainless steel jacket. The thermocouple junction is protected from the combustion products and radiation by two ceramic shields. A schematic of the probe is shown in Fig. 4. The probe tip was cast from alumina. It consists of a 16 mm outside diameter tube, 3 mm wall thickness, sealed at one end with ceramic. A circular opening, 10 mm in diameter, is located on top of the probe tip. This opening allows gas to be drawn into the probe around a smaller 6 mm diameter mullite sheath. The inner sheath, containing the thermocouple, is located behind this opening so that it is shielded from any direct radiation.

The principle of operation of the suction pyrometer is that at high enough velocities the convective heat transfer of the gases to the sheath will dominate over the radiative losses or gains from the surroundings. Therefore, the sheath will approach the gas temperature and the thermocouple will measure the sheath temperature. The manufacturer claims a ± 8 K accuracy. In order to ensure that adequate suction velocities through the pyrometer were maintained, the pressure inside the probe was kept below the reactor pressure. Keeping the opening clear from slag and coal particles was extremely difficult in the upper section of the reactor. The tip had to be changed after every four or five measurements due to clogging of the opening and deposition on the probe tip. However, tests showed
Fig. 4 - Schematic diagram of the suction pyrometer.
that as long as the opening was not completely blocked adequate flow through the suction tube was
maintained. The suction was provided by a Venturi nozzle hooked to an air supply with 1 MPa line
pressure. The pressure on the suction line exceeded the manufacturer's minimum specifications of 0.3
MPa. The nozzle produced a vacuum at the end of the suction hose allowing the hot gasses to be
extracted past the pyrometer's thermocouple. Blockage was detected by use of an on-line pressure gage
and by monitoring the temperature of the exhaust line. An increase in vacuum pressure or decrease in
exhaust line temperature indicated probe blockage. This required tip changes before additional
measurements were made.

Voltage readings from the S-type thermocouple were taken using a Fluke multimeter with accuracy
to ± 0.15 mV (± 14 K). A polynomial curve fit was used to convert the voltage readings to temperatures.
This conversion was accurate to within ± 1 K over the range of temperatures measured. Data were taken by
inserting the probe into each port and varying the radial positions from centerline to a position 35 cm out
from centerline. The positioning of the probe tip opening had an uncertainty of ± 1 cm. Measurements
were recorded after the probe reached steady-state. This took from 1 to 3 minutes to achieve. In the
visible flame zone there was never a true steady-state reading. The voltage measurements reached a
pseudo steady-state and then fluctuated by ± 0.3 mV (± 28 K). Outside of the visible flame zone (below
the first two ports) the fluctuations were only ± 0.1 mV (± 9 K). The overall measurement uncertainty was
estimated at ± 2.5% of the measured temperatures in the flame zone (a maximum uncertainty of ± 43 K).

2.3.2 Two-Color Pyrometer. A two-color pyrometer was used to measure local, particle-cloud
temperatures. Radiant emission measurements taken at two different wavelengths were used in
conjunction with the Planck distribution of blackbody intensity to calculate the particle cloud temperature.
The detectors in the probe were exposed to radiant energy centered around 1.27 and 1.60 μm. Incident
energy passed through filters with 30 nm bandwidths before being focused on the detectors. The
measured radiant energy came from a cylindrical control volume near the probe tip. The control volume is
approximately 4 cm in length and 4 cm in diameter. The water cooled probe consists of a detector housing,
sight tube and blackened target (see Fig. 5). The blackened, water-cooled target prevents contamination of the measurement from radiation outside the control volume of interest.

Before each series of tests the detectors were calibrated to ensure accurate temperature measurements. The calibration took place in a muffle furnace where a blackbody was heated to 1300 K and then allowed to cool to 900 K. The pyrometer was aligned to maximize the signals to the detectors. A thermocouple embedded in the blackbody reported detector temperature while the voltages from the detectors were measured. With these measurements, a calibration curve was obtained. Though the high temperatures experienced in the reactor could not be reached in the muffle furnace, the calibration curve was extrapolated out to higher temperatures by using a calibration constant and the manufacturer's calibration equation.

A full description of two-color pyrometry theory and data reduction is found in Butler (1992). The instrument determines the average particle cloud temperatures by measuring the radiant energy emitted at two wavelengths and using those measurements in conjunction with an approximation of Planck's energy flux distribution proposed by Wien (Eq. 1), where \( \lambda \) is the wavelength, \( C_1 \) and \( C_2 \) are constants and \( T \) is the temperature.

\[
E_\lambda = \frac{\tau_\lambda \varepsilon_\lambda C_1}{\lambda e^{\frac{C_1}{\lambda T}}} \tag{1}
\]

This equation is valid to within ± 1% of the Planck distribution over the range measured by the detectors. By assuming that the transmissivity (\( \tau_\lambda \)) of the particle cloud and the emissivity (\( \varepsilon_\lambda \)) of the particles are independent of wavelength (gray), the energies measured by each detector can be ratioed to solve for the particle cloud temperature (\( T_{pc} \)) shown in Eq. 2.

\[
T_{pc} = \frac{C_2 \left( \frac{1}{\lambda_2} - \frac{1}{\lambda_1} \right)}{\ln \left( \frac{E_{\lambda_1}}{E_{\lambda_2}} \right) + 5 \ln \left( \frac{\lambda_1}{\lambda_2} \right)} \tag{2}
\]
Fig. 5 - Schematic diagram of the two-color pyrometer.
The voltage readings from the two detectors are proportional to the detected energy from the particle cloud; therefore, the voltage ratio can be used in place of the energy ratio in Eq. 2. Other modifications made to Eq. 2 are the inclusion of a calibration constant (b) and a correction factor f which is a function of the detector temperature ($T_{dl}$). The temperature correction factor was necessary because the 1.60 μm detector's output was sensitive to changes in its temperature. Modifying Eq. 2 with these changes and inserting in values for $\lambda_1$ (1.60 μm), $\lambda_2$ (1.27 μm), and $C_2$ (14,388 mm K) leads to Eq. 3, where $T_{pc}$ is in Kelvins.

$$T_{pc} = \frac{2333.7}{\ln \left( \frac{V_{\lambda_1}}{V_{\lambda_2}} \right) + b}$$  \hspace{1cm} (3)

The calibration coefficient for these tests, $b=1.06$, was determined from testing in the muffle furnace. It compared well with the manufacturer's original calibration coefficient of $b=1.035$. The temperature correction factor based on data from the manufacturer and in-house testing is shown in Eq. 4.

$$f(T_{dl}) = 8.38 - 0.0588T_{dl} + 0.000114T_{dl}^2$$  \hspace{1cm} (4)

The detector's temperature ($T_{dl}$) was measured using a T-type thermocouple.

Sampling in the reactor occurred in much the same way as was done with the suction pyrometer. The probe was inserted at different axial locations and then radial profiles of particle cloud temperature were acquired. The position of the probe was determined from the centerline of the control volume. Therefore, a position 10 cm from the reactor's centerline actually contains information from 8 cm to 12 cm because of the 4 cm control volume length. For each measurement, the detector temperature was recorded and the voltage output was corrected using Eqs. 3 and 4. The detector temperature rarely varied by more than ±3 K. The voltages from each detector were sampled simultaneously using a sample-and-
hold device and a data acquisition board. The voltages were sampled at 100 kHz, much faster than the turbulent fluctuations in the reactor. Gain settings on the detectors were adjusted to prevent saturation of the data acquisition board, which saturates at inputs above 5 volts.

At each position where data were collected, 256 sets of 1000 data points were taken. Each set of 1000 points was averaged and recorded, requiring 0.25 seconds. The 256 averages were then analyzed to determine a mean particle-cloud temperature for that control volume. Average sampling time at each position was one minute. A time resolved data stream was also taken where 65,536 measurements were obtained. These data were sampled at 2 kHz and was streamed directly to disk without analysis. After sampling was complete, a post-processor program calculated time-resolved temperature measurements, mean and standard deviations of temperature, temperature fluctuation intensity \((T'/T_m)\), and power spectral density and probability density functions of temperature.

Uncertainty analysis was based on several factors that contribute to differences between measured temperatures and actual temperatures. These include scattering of light both in and out of the control volume, nongray behavior of the particles, soot emission, absorption, scattering, and temperature gradients in the control volume. Work by Lafollette et al. (1989), and Grosshandler (1984), has shown that soot volume fractions of up to \(10^{-6}\) in the flame region can give erroneously high temperature readings. These errors range from 150 K to 200 K. Temperature measurements are also weighted towards the higher temperature particles because the energy emitted is a function of temperature to the fourth power. With a 200 degree gradient at combustion temperatures Lafollette et al. (1989) reported up to 40 K higher measured mean temperatures than the actual mean. A more complete explanation of uncertainty analysis for the two-color pyrometer is given in Butler (1992). His analysis showed the uncertainty of measured mean particle cloud temperatures to be 80 K higher than the actual mean particle cloud temperatures outside of the reaction zone, and up to 200 K higher in the reaction zone (less than 30 cm from the quarl and 15 cm from centerline) for the probe used in this study.

2.3.3 Heat Flux Probes. Both water-cooled probes are 43 mm in diameter. During measurements the tips of the probes were aligned with the inside firewall of the reactor. They were left in position until
they reached a steady-state condition, usually within 3 minutes. The ellipsoidal radiometer (Butler and Webb, 1991; Butler, 1992) shown in Fig. 6, measured all incident radiation from a $2\pi$ steradian solid angle by converting the radiant heat flux into a millivolt potential across a differential thermocouple. Its hollow gold coated ellipsoidal cavity has a 3 mm aperture at one focus and a detector at the other. The total heat flux meter (see Fig. 7) measured combined convective and radiative heat flux. The incident heat flux to the stainless steel plug induced a temperature difference between the exposed end and the water-cooled back of the plug. This temperature difference between two points located along the plug axis was calibrated to determine the total heat flux.

Repeated tests and measurements supported the manufacturer's claim of accuracy to within ± 5% of the measurement for both probes. Variations in wall temperatures due to the opening and closing of access ports raised total uncertainty to approximately ± 10%. It should be noted that the measurements of heat flux to the walls are not the same as the heat flux to the probe due to the temperature difference between the hot walls and the cool probe. Because of this temperature difference, there is a higher heat flux to the probe than to the walls. In fact, convective heat transfer can occur where hot walls heat the cooler combustion gasses.

From the total and radiative heat flux measurements the convective heat flux to the reactor walls was calculated. These calculations were determined using a data reduction scheme developed by Butler (1992). The convective heat flux to the probe is equal to the difference of the total and radiative fluxes measured by the probes. Using these data a convective heat transfer coefficient to the probe was calculated. By using data from both gas and wall temperature measurements, a convective heat transfer coefficient for the walls was also calculated. This new coefficient was used to calculate the convective heat transfer to the walls. The radiative heat flux plus the convective heat flux to the walls is the total heat flux to the walls.

2.3.4 Particle Counter Sizer Velocimeter Probe (PCSV). Particle size, velocity and number density in the CPR were measured using the PCSV manufactured by Insitec Measurement Systems. The PCSV instrument is a single particle counter capable of measuring particle sizes from approximately 0.5 μm
Fig. 6 - Schematic diagram of the ellipsoidal radiometer.
Fig. 7 - Schematic diagram of the total heat flux probe.
to 100 μm and particle velocities from near zero to several hundred meters per second. A schematic of the probe (PCSV-P) used in the CPR is shown in Fig. 8.

Particle size measurements are done by measuring the maximum amplitude of the Gaussian-shaped scatter signal in the near forward direction (approximately 5 degrees) of each individual particle as it passes through the sample volume of the instrument. The PCSV is a single particle counter and therefore operates on the restriction of single particle scattering. This means that the instrument can operate in flows with number densities such that only a single particle passes through the measurement volume at a time. Using a small collection angle minimizes the scattering signal sensitivity to particle shape, as shown by Orfanoudakis and Taylor (1992). The response function which relates the maximum amplitude of this signal to the particle diameter is based on Lorenz-Mie theory. A deconvolution algorithm is incorporated into the calculation of the particle diameter to account for the Gaussian intensity profile of the sample volume. This procedure corrects for the directional effects of the particle trajectory on the measured diameter. Particle velocities are measured by determining the time of flight of the particle across a known sample volume. Reported velocities represent mean values for all the particles passing through the sample volume in the small and large size classes.

The PCSV-P uses two beams for particle size and velocity measurement to expand the number density operational range. These are referred to as the large and small beams. The small beam measures size and mean velocity for particles from 0.5 to 2 μm, the large beam measures the sizes and mean velocities of particles from 2 to 100 μm. Larger beam waists allow measurement of larger particles, however, at the same time the number densities where the instrument can operate is lowered due to the single particle restriction on the sample volume. The particular instrument used in this study has a large beam waist of 190 μm and a small beam waist of 19 μm. This makes the measurable size range approximately 0.5 to 100 μm with a number density limitation of 10^6 particles/cm^3. The theory of the PCSV technique is describe in detail by Holve and Self (1979), Holve (1980, 1982), and Bonin (1992).

Calibration is done with a reticle disk which simulates various particle sizes over the measurement range of the instrument. The calibration reticle is a coated disk with circles of various diameters etched on
Fig. 8 - Schematic of the PCSV-P.
it. The etched holes simulate diffraction of a given particle size since diffraction is primarily an edge effect. Calibration tracks consist of particle sizes of 2, 5, 10, 20, 40, and 80 \( \mu \text{m} \).

The probe, as shown in Fig. 8, is placed inside a cooling jacket leaving only the flow window exposed. This assembly is then inserted in CPR. The probe is positioned radially in the reactor and then rotated to align the flow window of the instrument with the reactor's swirling flow. Aligning the flow passage with the mean flow direction minimizes possible errors resulting from the establishment of recirculation zones inside the instrument's flow window. The alignment procedure is done by rotating the probe until the maximum particle data rate is observed. In practice, due to the intrusive effects of the probe, the data rate remained fairly constant over 5 to 10 degrees of rotation. The correct angle was taken to be approximately the center of this range.

Laser power levels for each beam were determined at the beginning of every measurement to account for any decrease in laser power over time. This procedure accounts for the effect of any particle deposition on the flow window. Data could be taken successfully until power levels dropped to about 50% of the calibration levels, then the probe was removed from the reactor and the windows cleaned. Beam powers lower than 50% of the calibration are not used since the amplitude of the scattered signal from the small particles decreases to a point where accurate measurement of the scattered light is not feasible. Also, the possibility of beam broadening was present. This occurs in high number density flows where the baseline scattered signal is lifted. The amplitude of the scattered signal then becomes more distorted as power levels fall. Therefore, beam power levels are kept relatively high to minimize this effect.

Sampling times used in the CPR varied depending on location. In locations of high number density, relatively short sample times were needed compared to lower sections where number densities were low. Sampling times were determined from preliminary measurements taken prior to the final test runs. The amount of time needed for a measurement at a given location in the CPR was found by taking several samples at this location and determining the measurement time needed so that the results from different measurements at the same location were within the error of the instrument. Final measurements were taken at axial locations of 30, 70, and 150 cm from the quarl. However, the measurements taken 70
cm from the inlet exhibited erratic behavior due to destruction of the recirculating flow field in the CPR caused by the large diameter of the probe.

Estimates on the error associated with the particle velocity and size measurements are based on the manufacturer's claims (the manufacturer's specified error bounds are ± 10% of the measured particle size) and past work on probe intrusion error in the CPR done for a previous study by Bonin (1992). Error is also introduced because of particle deviations from sphericity, changes in particle refractive index during the combustion process, and sampling statistics. These issues are discussed by Bonin and Queiroz (1994) specifically for measurements with the PCSV in reacting pulverized coal environments. Bonin and Queiroz estimate errors in the particle-size measurement associated with the non-sphericity of the particles and variations in refractive index to be small, on the order of 5%.

Probe intrusion effects are another large source of error when applying the PCSV-P to the CPR. In a similar study done previously in the CPR, Bonin (1992) showed that velocity errors due to probe intrusion ranged from 20% to 40% depending on location in the reactor. The high degree of probe intrusion is due to the relative size of the optical probe and its cooling jacket (8 cm) compared to the inside diameter of the reactor (80 cm).

From the above discussion, measurement accuracy can be estimated to be between 20 to 40%, due to the geometry of the CPR, the nature of the particulates, the size of the probe, and the harsh reacting environment. The previous work on the error of the PCSV in the CPR shows that error is high in the upper ports where the gradients are large and the swirl is more intense. At lower ports accuracy is improved. Although large errors are present when using the PCSV technique in the CPR, the PCSV-P instrument provides valuable information on the order of magnitude of particle number densities and velocities in-situ in the reactor. This type of instrumentation is currently the only means of obtaining this type of data for nonspherical particles such as pulverized coal.

2.3.5 Transmissometer. Monochromatic transmission was measured by passing a laser beam across the diameter of the CPR at various axial positions. The entire diameter of the reactor was used as the diagnostic volume so that a significantly detectable beam extinction could be measured. A 10 mW helium-
neon laser operating at a wavelength of 632 nm was used as the light source as shown in Fig. 9. A high-speed photodetector collected the transmitted light at a sampling rate of 2 kHz. Several sets of 131,072 measurements were collected at each axial position. A 12-bit analog-to-digital board was used to collect detector voltages. The aperture on the receiving end limited the forward solid angle to a known size for scattering calculations. An optical narrow bandpass filter centered on the laser frequency was used at the detector.

Spectral transmissivity through the diagnostic volume of the CPR was derived using Beer’s law:

$$\tau_\lambda = \frac{I_{\lambda,L}}{I_{\lambda,0}} = e^{-\kappa_\lambda L}$$  \hspace{1cm} (5)

where $I_{\lambda,L}$ is the measured beam intensity after passing through the absorbing medium, and $I_{\lambda,0}$ is the beam intensity measured with no particles in the beam path. The voltage output of the detector varied linearly with incident intensity from the laser so that the following relationship held:

$$\tau_\lambda = \frac{I_{\lambda,L}}{I_{\lambda,0}} = \frac{V_L}{V_0}$$  \hspace{1cm} (6)

This allowed direct calculation of transmissivity from detector voltage measurements. Mean and standard deviation voltages were calculated for each set of data, then the mean voltage was used in Eq. 6 to calculate transmissivity.

The largest source of potential error in the measurements was laser beam power drift. Baseline beam powers were established by moving the apparatus away from the reactor and gathering a small data set before and after collecting data in the reactor at each axial position. Beam power was weakly dependent on ambient temperature, but maximum drift was measured at ± 0.1 volts over the 5 volt range of the detector. Detector saturation was avoided by closely monitoring the baseline powers throughout the test sequence. Background noise in the photodetector was measured by capturing a data set without any outside radiation impinging on the detector face. Maximum variation in the signal was ± 1 mV out of a
Fig. 9 - Experimental transmissometer setup.
potential 5 volts. Emission from the flame was another possible source of uncertainty and this was quantified by blocking the laser and allowing the detector to pick up any emission from the flame or surroundings. Variations in the signal using this approach were limited to ± 2 mV due to the narrow bandwidth of the optical filter.

Accurate transmission measurements required that the path length through the particle flow remain constant and known throughout all of the tests. Some fluctuation of the path length was noted during the tests due to variations in reactor pressure. With increased reactor pressure, some particles would be forced out of the reactor ports along the path of the beam. These fluctuations were very brief, and would increase the path length by approximately 2-4 cm out of the 80 cm reactor width, or a maximum of 5%. The brevity of the disturbances gave a total uncertainty in the mean transmission of less than 3%.

2.3.6 Gas and Solid Sampling Probe. Solid and gas samples were collected from the reactor with a small probe and collection system shown in Fig. 10. The isokinetic probe extracts samples from the reactor at the same velocity as the flow in the reactor, so that smaller particles do not bypass the probe, or are drawn in preferentially. It consists of two parallel tubes: one that supplies deionized water to the probe tip, and one that suctions off this water mixed with gas and solid sample. The probe inlet pressure was changed by adjusting the water flow into the probe. This allowed the sample velocity entering the probe to approximate the free stream velocity, so the sample would be representative of the actual gas and particle mixture in the reactor. The probe was always oriented so that the opening pointed towards the top of the reactor.

Solid and gas samples drawn into the probe were quenched with a water spray at the probe inlet to freeze the reactions. The inlet water spray was maintained at 650 ml/min. The sample proceeded through an ice bath to condense water vapor. A water trap then separated the particles and water from the gases. The contents of the trap were drained, labeled and stored. The gases passed through the oil-less diaphragm vacuum pump to the Lancom 3400 portable gas analyzer. The Lancom 3400 used chemical cells to measure quantities of NO\textsubscript{x} and O\textsubscript{2} in a gas mixture. The measurement uncertainty reported by the manufacturer was ± 1% for O\textsubscript{2} and ± 4% for NO\textsubscript{x}. 
Fig. 10 - Schematic diagram of the isokinetic sampling system.
The water-particle mixture removed from the trap was passed through a 2.7 \textmu m filter to collect the particulates. The samples were then dried in a drying oven. Multiple 6 mg samples from each reactor location were analyzed in a Leco CHN 800 analyzer to determine percentages of carbon, hydrogen and nitrogen in the sample. The analyzer was reported by the manufacturer to have an uncertainty of \( \pm 0.3\% \) in the carbon measurement and \( \pm 3\% \) for nitrogen concentrations above 1\%. Concentrations of nitrogen below 1\% had an absolute error of \( \pm 0.03\% \), while concentrations of hydrogen had an absolute error of \( \pm 0.02\% \).

The solid sample concentrations of carbon were used to calculate carbon burnout. Carbon burnout (\( B_{cb} \)) was defined as:

\[
B_{cb} = 1 - \left[ \frac{X_{cb,s}}{X_{a,s}} \frac{X_{cb,cl}}{X_{a,cl}} \right]
\]

where \( X \) represents the mass fraction of the material. The cumulative burnout for carbon, hydrogen, and nitrogen species was calculated using Eq. 8.

\[
B_1 = 1 - \left[ \sum_{i=1}^{n} \frac{X_{i,s}}{X_{a,s}} \frac{X_{i,cl}}{X_{a,cl}} \right]
\]

Carbon, hydrogen, and nitrogen represent the \( i^{th} \) species shown in Eq. 8.

The remaining dried sample was then weighed, completely burned in a furnace, and weighed again according to ASTM D3174-89 procedure (ASTM, 1989). Total burnout was then calculated using the following expression:
\[ B_t = 1 - \frac{\left[ \frac{1 - X_{a,s}}{X_{a,s}} \right]}{\left[ \frac{1 - X_{a,cl}}{X_{a,cl}} \right]} \]  

The ultimate analysis information was used in calculating both carbon burnout and total burnout.

Samples were taken at 34 different locations throughout the reactor at various axial and radial locations. Measurements were concentrated in the upper ports near the reaction zone. Steps were taken throughout the test to ensure that no air leaks were present in the suction lines.
3. EXPERIMENTAL RESULTS AND DISCUSSION

In this section data from the CPR tests are presented. A discussion of the data collected by each instrument is given together with an analysis of the information with respect to measurements made with the other instruments.

3.1 Gas Temperature

Data were taken at seven different axial locations ranging from 15 to 190 cm from the quarl. At each axial position a radial profile was taken. Gas temperature measurements presented in Fig. 11 show that there is a decrease in centerline temperature as distance from the quarl increases. It is interesting to note that the radial profiles are basically flat at axial distances greater than 55 cm from the quarl. These locations are outside the luminous flame region. At all axial positions, radial temperature profiles show a sharp drop from the 30 cm to the 35 cm from centerline measurement. This could be the result of quenching effects near the wall or small leaks from the port opening contaminating the measurements. Measurements near the edge of the reactor also showed sensitivity to variations in reactor pressure. Another interesting observation is the decrease in gas temperatures of the 15 and 30 cm axial profiles as the radial distance from centerline increases. This decrease occurs outside the flame zone and may be caused by quenching effects of the reactor ceiling or by flow recirculation zones. This effect is not present at the axial locations lower in the reactor where the profiles are basically flat.

3.2 Particle Cloud Temperature

Mean particle cloud temperature measurements shown in Fig. 12 were obtained using the two-color pyrometer. Initially, the coal particles are radiatively heated as they enter the reactor. The coal particles devolatilize and ignite as they reach the fire ball and form a visible reaction zone. This bright reaction zone occurs near the quarl in the upper 30 cm of the reactor. The lower centerline temperatures in the upper two ports indicate that the particles are still heating and have not reached the flame front as they pass through the central portion of the reactor. The profile in Fig. 12 at an axial position 15 cm from the quarl shows particle temperatures along the centerline being 100 K lower than those measured for
Fig. 11 - Radial gas temperature profiles measured by the suction pyrometer.

Fig. 12 - Radial particle cloud temperature profiles measured by the two-color pyrometer.
locations further out from the centerline. The radial profile at 30 cm from the quarl shows similar trends with a 50 K difference. However, the centerline temperature at 30 cm is hotter than the centerline temperature at 15 cm due to its proximity to the flame zone. Peak gas temperatures and visual observations also indicate that the flame front is slightly shifted by 2 cm to the north side of the reactor (see Figs. 3 and 11). These trends along with visual observations support the diagram of flame position shown in Fig. 13. The particle cloud temperature reaches a maximum of approximately 1400 K in the region of the estimated flame front and then decays with increased axial distance from the flame ball. The flatness of the particle cloud temperature profiles outside the flame zone and the flatness of the gas temperature profiles in the lower port suggest that the particles are being uniformly cooled by radiation losses to the wall.

Since the detectors in the two-color pyrometer are exposed to all the particles in the control volume and the probe is measuring a turbulent flame, there are temporal temperature fluctuations in the particle cloud. A measure of those fluctuations is the standard deviation from the mean. The standard deviation was computed for the 256 averages, each consisting of 1000 data points taken over 1 msec (see Fig. 14).

As expected the highest standard deviations occur in the measurements near the fire ball. These measurements have standard deviations that approach 60 K. At the second port, the standard deviation is about half of that at the first port. The standard deviation in temperature decreases in the lower ports to 15 K and continues to decrease to 4 K near the bottom of the reactor. The profiles for standard deviations are flat more than 30 cm below the quarl. The lack of visible reaction and the decrease in turbulent fluctuations in the lower portions of the reactor cause the particle cloud to reach a temperature profile that is insensitive to radial variation and is constant at a given axial distance from the bottom of the quarl.

The number of measurement locations where stream data were taken by the two-color pyrometer was not as extensive as the number of locations where averaged data were taken. The mean temperatures of the streamed data are shown in Fig. 15. The mean temperature measurements are reasonably close to those of the averaged values in Fig. 12, showing smooth radial profiles at 70 and 150 cm from the quarl and showing the increase in temperature as the particles approach the flame zone in the port 30 cm from the quarl. The one difference in the data is the centerline temperature of the top port. This difference could
Figure 13 - Estimated flame position in the reactor.
Fig. 14 - Standard deviations of the average particle cloud temperature.
be caused by the turbulent nature of the flame or slight flame shifts. A comparison between the standard deviations of the stream data temperatures (Fig. 16) and the averaged standard deviations (Fig. 14) shows remarkable similarities. The profiles have the same trends and magnitudes. Temperature fluctuation intensity measurements ($T'/T_m$) followed the same trends as the standard deviations. The maximum turbulent intensity of 4% occurred at the top port, this dropped to 2% at the second port and then below 1% for the rest of the reactor. The analysis of the power spectral density functions revealed no dominant frequency of temperature fluctuations.

An analysis was done to determine if the temperature distributions were Gaussian. In Fig. 17 the centerline temperature distribution, shown in the form of a probability density function, reveals that the distribution is skewed to the higher temperatures in the upper ports and then approaches a Gaussian distribution at the lower ports of the reactor. This skewness of the graphs towards the higher temperatures in the upper port may be a function of the higher emissions from higher temperature particles. There is a marked difference in the temperature spread as a function of axial distance from the quarl. At the top there is a variation in temperature of more than 150 K, in the middle of the reactor the spread is 30 K and it drops to 20 K at the bottom of the reactor. The axial variation in centerline trends are representative of the axial variations at extended radial positions.

3. 3 Total, Convective, and Radiative Heat Fluxes

The measurements of total, convective, and radiative heat fluxes in the reactor are shown in Fig. 18. Data shown are representative of multiple measurements made throughout the testing periods. The graph of total heat flux shows the combined convective and radiative transfer to the probe. A constant total heat flux for the top three ports is followed by a smooth decay as axial distance from the quarl increases. The radiative measurements show a constant decay of radiative heat flux with increased separation distance from the quarl. These measurements are consistent with other measurements and visual observations. The convective part of the total heat flux is a function of the gas velocity and the temperature difference between the gas and the probe. Near the wall, where the measurements were taken, the gas temperature reaches a maximum at the third port. The flow field at this point provides high
Fig. 16 - Standard deviations of the average particle cloud temperature using stream data.

Fig. 15 - Radial particle cloud temperature profiles using stream data from the two-color pyrometer.
Fig. 17 - Probability density functions of the centerline temperature distributions at various axial locations in the reactor.
Fig. 18 - Radiation, convection and total heat flux measurements as a function of axial positions in the reactor.
velocities to enhance heat transfer. Therefore, the convective heat flux reaches a maximum at this port and then decreases as the gas temperature decreases. The radiative heat flux is nearly independent of the gas temperature for this small reactor. It is only affected by the particle and wall temperatures. At the top port (15 cm below the quarl), the reaction zone is in direct line with the probe. The reaction is so intense that the medium is optically thick in the visible and the probe is effectively shielded from the far wall of the reactor. Therefore, it only measures heat flux from the hot reaction zone. At the lower ports, the reaction zone is not optically thick, causing most of the incident radiative flux to come from the reactor walls. Since the reactor walls decrease in temperature with increased distance from the quarl, the radiative flux to the walls also decreases. The flat zone of almost constant total heat flux in the top three ports is a result of the above-mentioned observations. The convective heat transfer increases in the top three ports are offset by the decreases in the radiative heat transfer. Below port 3, the lack of visible reaction and the cooler wall temperature cause an overall decrease in heat flux to both probes.

The heat flux absorbed by the wall is different than the heat flux absorbed by the probe. The probe temperature is kept near 30°C, while the average wall temperature varies linearly from 1300 K at the top of the reactor to 1100 K at the bottom of the reactor. This change in temperature gives rise to a large difference in the magnitude of the convective heat flux to the wall and to the probe. This can be seen by the difference between the line showing total heat flux to the probe and total heat flux to the wall. In the top of the reactor the wall temperature was hotter than the gas temperature causing convective heat transfer from the walls to the gas. This appears as a slight negative convective heat transfer to the walls. As can be seen in Fig. 18, the total heat flux to the walls is almost identical to the radiative heat flux. This indicates that heat transfer within the reactor is dominated by radiation.

### 3.4 Particle Size And Velocity

Figure 19 shows the cumulative number density information for the 1-1, 10, and 20 μm size classes while Fig. 20 shows the average velocities for the large (> 2 μm) and small (< 2 μm) particles at two axial positions in the CPR. Comparing the particle temperature and number density data plotted in Figs. 12 and 19 shows that the regions of highest number density correspond to the combustion zone located
Fig. 19 - Cumulative particle number densities in the CPR.
between 5 and 15 cm from the centerline at an axial position 30 cm below the quarl. Large particle velocities are consistently slightly higher than the small particle velocities for all the measured radial profiles. This is caused by the large particles having a higher inertia and failing to follow the turbulent fluctuations in the flow as well as the smaller particles. This gives them a slightly higher mean velocity.

As expected the gradients in both velocity and number density are highest in the upper ports in the reactor close to the inlet and become smaller further down in the reactor. Decreases in the particle concentrations with increasing axial location in the CPR is more pronounced for the 10 and 20 µm particles than for the 1.1 µm particles shown in Fig. 19, due to the reduction in the particle size as the particles burn out. Variations in the radial profiles of the volume mean diameters, shown in Fig. 21, are also greatest in the top of the reactor with the largest measured diameter of 35 µm corresponding to the approximate flame location. As axial location in the CPR increases, the gradients in the radial direction become smaller and the overall mean size of the particles decrease. At a distance of 150 cm the volume mean is approximately constant at 8 µm. Comparisons of data from several other measurements done at the same experimental conditions show considerable fluctuations in the particle sizing data. However, these differences were within the level of error expected for the PCSV-P measurements in the CPR as described previously in section two.

Concentrations measured during this study were considerably lower than those found in previous measurements done in the CPR by Bonin (1992). His work showed particle concentrations approximately twice those reported here. The particle sizes were also large with significant particles in the 30 µm range. These variations can be contributed the large differences in test conditions and coal type between the two sets of measurements. The measurements taken by Bonin (1992) were done using a Utah Blind Canyon coal, which produced an entirely different flame structure from the one produced from the Pittsburgh #8 coal used in this work.

3.5 Transmission

The transmission results for each axial position in the CPR are shown in Fig. 22. The increase in transmission with increasing axial distance in the reactor is consistent with the information observed in
Fig. 20 - Large and small particle velocity profiles.

Fig. 21 - Sauter and mass mean diameters of the coal particles.
Fig. 22 - Transmission measurements across the reactor using the transmissometer.
other measurements. Particle information taken with the PCSV, shown in Fig. 19, shows decreasing concentrations of particles corresponding to the observed increase in transmission. This is especially true for the larger particles in the size distribution which would have a tendency to scatter more light and thus have a larger impact on the transmission measurements made across the reactor. As the coal particles react some of their solid volume is transformed into gaseous fuel causing a smaller volumetric cross section resulting in less attenuation of the transmitted signal as shown in Fig. 22.

3.6 Species Concentrations And Particle Burnout

Measurements of gas and particle species and burnout were not originally included in the proposal submitted to DOE. These measurements were taken, however, to add completeness to the data sets. Testing of CO concentrations was not possible due to instrumentation problems with the CO gas cell in the gas analyzer. This additional information would have been helpful in confirming burnout measurements and reported stoichiometries. The other information presented does give additional insight in the areas of NOx formation, burnout and oxygen concentration.

The minimum measured carbon burnout percentage is 65% at a position 15 cm below the quarl, (see Fig. 23). This shows that a good portion of the combustion has already taken place in the quarl above where probe access was possible. The carbon burnout values are progressively higher as axial separation from the quarl increases, showing continued reaction outside the visible flame zone. Near the exit of the reactor the burnout profile is very flat, near 90%. This high value of burnout considering the stoichiometry may be indicative of incomplete combustion resulting in high CO levels. Figures 24 and 25 show total burnout calculated by two techniques: 1) the ASTM standard; and 2) a technique based on the CHN analysis. Comparisons show higher total burnout than that of the carbon burnout. This gives a strong indication that devolatilization and not char oxidation occurred in the quarl section.

The carbon present in the extracted solids is shown in Fig. 26. These measurements were used in calculating the carbon burnout data as described in subsection 2.3.6. Hydrogen and nitrogen in the solid samples are shown in Figs. 27 and 28. These figures show that devolatilization occurs high in the reactor. The original hydrogen content is 5.15% in the coal. The first port centerline measurement of
Fig. 23 - Percent carbon burnout measured by ASTM technique.

Fig. 24 - Total burnout measured using the ASTM technique.
Fig. 25 - Total burnout calculated using the CHN data.

Fig. 26 - Carbon percentage in the extracted solids.
Fig. 27 - Hydrogen percentage in the extracted solids.

Fig. 28 - Nitrogen percentage in the extracted solids.
3.8% is the only value that even approaches the original content. The measurements below port 1 are almost all below 0.5%. From this it can be concluded that most of the hydrogen is released as volatiles. The nitrogen content decreases slowly as the axial distance from the quarl increases. This indicates that it is being released as the char is being oxidized and not rapidly during devolatilization as was the hydrogen.

Oxygen measurements in Fig. 29 show progressively lower oxygen levels as the gases move away from the quarl. Along the centerline at port 1, the oxygen level is at 13%, indicating that 38% percent of the initial oxygen has been used in combustion while in the quarl. The rapid decrease in oxygen quantities in the top two ports between the centerline and 15 cm support the postulated flame position shown in Fig. 13 and concur with the other data taken during these tests. The presence of 1-3% oxygen in the bottom quarl may be due to incomplete combustion or air leakage into the reactor through the testing ports.

Figure 30 shows NOX levels in the reactor. The peak value of NOX attains levels just below 1000 ppm. This peak value corresponds to the position of the flame front indicating NOX formation as the coal passes through the visible reaction zone. The low measurements of NOX at the top two ports near the centerline support this hypothesis. Average NOX concentrations even out to approximately 650 ppm throughout the reactor below port 3. The lack of appreciable increase in NOX concentrations below port 3 indicate that the fuel nitrogen is not being transformed into NOX outside of the flame front region.

3.7 Conclusions. A complete data set of gas and particle parameters was provided at the conditions shown in Table 1 for a pulverized-coal flame. Data presented includes: gas, particle, and wall temperature profiles; radiant, total, and convective heat fluxes to the walls; particle size and velocity profiles; transmission measurements; gas species concentrations; and carbon and total burnout. Sharp gradients in temperature and species concentrations were evident in the upper sections of the reactor where the reaction zone was located. Measurements showed that devolatilization occurred high in the reactor, however, char oxidation continued throughout the region investigated.
Fig. 29 - Oxygen distribution measured by the suction probe and Lancom 3400 gas analyzer.

Fig. 30 - NO\textsubscript{x} distribution measured by the suction probe and the Lancom 3400 gas analyzer.
4. COMPREHENSIVE CODE SUB-MODEL EVALUATION

4.1 Particle Dispersion Modeling

The objective of this section is to study parametrically the predictions of a particle dispersion submodel incorporated in a commercially available, comprehensive, 2-dimensional, pulverized-coal combustion and gasification code known as PCGC-2. This code is available at the Advanced Combustion Engineering Research Center (ACERC) located at Brigham Young University (Smoot et al., 1988). The experimental data used to study the predictive capability of this submodel were obtained in the laboratory-scale, axisymmetric, Controlled-Profile Reactor (CPR) using a laser-based instrument (Bonin, 1992).

4.1.1 Model Description. The approach used in PCGC-2 is based on the Particle-Source-In Cell (PSI-CELL) technique of Crowe et al. (1977). This model is based on calculating the trajectories of representative particles through the gas-phase (continuum) field in a Lagrangian fashion. Mean particle velocities, trajectories, temperatures, and compositions are obtained by integrating representative equations for the mean motion, energy and component continuity for an ensemble of particles in the gas-flow field. The net difference in the particle properties leaving and entering any cell then provides the particle source terms for the gas-phase equations. Care is taken to account for all modes of gas-particle coupling. The method does not account for all modes of particle-particle interactions and thus would not apply to highly loaded, dense flow.

The particle momentum equation for a single ($i^{th}$) particle in the Lagrangian framework is given by:

$$\alpha_j \frac{d}{dt}(\vec{v}_j) = \vec{f}_j + \alpha_j \vec{g}$$

where $\alpha$ is the mass of the particle, $\vec{v}$ is the velocity vector, $\vec{f}$ and $\vec{g}$ are the drag and body force terms, respectively.

The properties used to evaluate Eq. (10) are the time-mean gas properties. Therefore, the diffusion effect due to turbulent fluctuations is not accounted for; i.e., the equation is deterministic in
nature. In order to account for turbulent diffusion, the diffusion velocity is superimposed on the convective velocity; i.e., the particle velocity is decomposed into convective (deterministic) and diffusive components:

\[ \vec{v}_j = \vec{v}_{jc} + \vec{v}_{jd} \]  

(11)

The convective component \( \vec{v}_{jc} \) is defined as the velocity that would arise in the absence of turbulence, or the ballistic velocity based on the mean gas velocity. It is obtained from the solution of Eq. (10) using time-mean gas properties. The diffusive component \( \vec{v}_{jd} \) of the velocity is modeled using a gradient diffusion approximation (Baxter, 1989; Jurewicz and Stock, 1976; Faeth, 1983):

\[ \vec{v}_{jd} \bar{n}_j = -D_j \nabla \bar{n}_j \]  

(12)

where \( D_j \) is the transport coefficient, which in this case is called the turbulent particle diffusivity, and \( \bar{n}_j \) is the average particle number density. The turbulent particle diffusivity can be expressed as the ratio of the turbulent particle kinematic viscosity and the turbulent particle Schmidt number. The turbulent particle kinematic viscosity can be obtained from the expression of Melville and Bray (1979). However, an empirical value of the turbulent particle Schmidt number is needed in order to solve for the diffusion component of the particle velocity. Also note that \( \bar{n}_j \) cannot be calculated from the Lagrangian particle-phase information, and can only be approximated using the Eulerian gas-phase information. The procedure used is to formulate the transport equation for the mean particle number density and solve it after the gas phase calculations. Further details of this model can be found in Smoot et al. (1988).

4.1.2 Model Evaluation. The details of the experimental and numerical test conditions are presented in Shirolkar and Queiroz (1993). The simulation results presented below are for the reacting base case. For this test condition the experimental swirl number, equivalence ratio, coal flow rate (kg/h), secondary air flow rate (kg/h), and mass-mean particle size (\( \mu m \)) were 1.4, 1.15,
11.4, 126.0, and 55 respectively. The coal-type used in the experiments was the Utah Blind Canyon coal. The different coal properties required as input conditions for the simulations is also presented in Shirolkar and Queiroz (1993).

The particle dispersion submodel calculates the mean trajectories representing a particular size originating from a specified initial starting location inside the primary inlet. The number of starting locations inside the primary inlet was fixed at the maximum value of 10 for the present geometry. It was also found that by increasing the number of discrete particle sizes representing the input, coal-size distribution beyond 10 sizes did not change the dispersion predictions significantly. Therefore, during each particle iteration 100 trajectories were simulated. Also a Schmidt number of 0.35, which is known to give reasonable results when used in PCGC-2 (Fletcher, 1983), was used for all simulations. Further details of these simulation parameters (grid size, number of initial particle sizes, and Schmidt number) can be found in Shirolkar (1992).

Sloan (1985) studied the performance of the k-ε model, which is used for the turbulent gas-flow predictions in PCGC-2, for strong swirling flows. His results indicate that the prediction of the k-ε model is generally poor in the near burner region. Simulations performed by Costa et al. (1990) for a swirling pulverized-coal flame also indicated the predictive deficiency of the k-ε model in the near burner region. However, they managed to obtain relatively better predictions by reducing the swirl number for the simulation. Since the particle dispersion model is coupled with the gas-phase equations, any deficiency in gas-phase predictions will affect the dispersion predictions. Therefore, in order to establish the effect of employed swirl number on gas-flow predictions as well as on the dispersion statistics, simulations were performed for two different swirl numbers. The swirl numbers used for these simulations included the experimentally measured swirl number of 1.4 and a reduced swirl number of 0.8. The reduced swirl number of 0.8 was selected after extensive investigations which involved comparisons of predicted gas and particle velocities, particle number densities and gas temperatures with experiments.

General Aerodynamics. Figures 31 (a) and (b) show the predictions of gas flow pattern along with the particle trajectories for swirl numbers of 1.4 and 0.8, respectively. For the purpose of simulation, the particle and gas velocities were assumed to be the same at the reactor inlet. These plots show that the
Fig. 31 - Predicted velocity vectors and particle trajectories for reacting base case using a swirl number of (a) 1.4 and (b) 0.8.
main features of the flow predictions are a strong internal reverse-flow zone (induced by the swirl imparted to the secondary air) and an external recirculation zone (caused by the sudden enlargement of the furnace chamber). The strength and size of the internal, reverse-flow zone predicted by the k-ε model for a swirl number of 1.4 is definitely greater compared to those predicted using a swirl number of 0.8. This results in a relatively less penetration of the primary jet containing the coal particles into the internal reverse-flow zone for the higher swirling case. The predictions show that for both cases the particles are dispersed toward the reactor wall with relatively greater dispersion observed for the higher swirling case. This is substantiated by significant ash deposition on the reactor wall observed during experiments. There appears to be no significant difference between the external recirculation zones predicted for the two cases (Figs. 31 (a) and (b)).

The first set of comparisons between the experimental data and the predictions consists of comparing the small particle (0.4-3.5 μm) velocity experimental data with the gas axial velocity predictions. Such comparisons are possible because the small particles are expected to follow the gas flow due to their lower inertia and free-fall velocity. In the experiments, the laser based, Particle-Counter-Sizer-Velocimeter (PCSV) probe was rotated through a known angle to align the flow channel of the probe with the mean flow, it was necessary to calculate the axial velocity component in order to carry out these and any further velocity comparison with the predictions.

Figures 32 (a) and (b) show the comparisons between the experimental small particle axial velocity with the gas-phase velocity predicted for swirl numbers 1.4 and 0.8 at two different axial location (x = 0.3 m and x = 1.9 m). The axial location x = 0.3 m is around the penetration zone whereas the axial location x = 1.9 m is at a location further downstream. It is evident from Figure 32 (a) that predictions for the two different swirl numbers differ significantly in a region close to the reactor centerline. As for the comparison with the experimental data, the lower swirl number case (0.8) appears to agree with the experiments from the centerline up to a region just before the predicted gas flow reverses its direction. It should be noted at this point that the PCSV probe was intrusive in nature and was not capable of recording velocities in the reverse direction. It is difficult to characterize the impact of the probe on the flow inside the CPR. However, Bonin (1992) studied the isothermal gas-phase velocity with a hot film anemometer with and without the
Fig. 32 - Comparison between the predicted gas axial velocity and the experimental data for small particle velocity for two different simulation swirl numbers (1.4 and 0.8) at axial distances of (a) 0.3 m and (b) 1.9 m.
PCSV probe in the flow for both swirling and non-swirling flows. His results showed that the impact of the probe intrusion on gas-phase velocity measurements can reach as high as fifty percent, especially in the near burner region for the swirling case. Due to the complex flow structure that develops with the introduction of the particle-phase, it is difficult to assess the implications of the hot film characterization relative to the PCSV measurements of particle velocity. At best, the hot film investigation provides an indication that there may be a considerable effect of probe intrusion in the near burner region, i.e., the internal reverse-flow zone. Therefore, the probe intrusion and the inability of the probe to record negative velocities is an important factor to consider while making such comparative evaluations. The axial location of \( x = 0.3 \) m is outside the penetration zone and within the internal reverse-flow zone for the swirl number of 1.4; hence its predictions differ very significantly from those observed experimentally. This observation suggests that the primary jet penetration could be underpredicted for the swirl number case of 1.4. Figure 32 (b) shows that the experimental data and the predictions for both cases relate fairly well further downstream. This is a region where there is no reverse flow for a swirl number of 0.8 and a small region of reverse flow near the centerline for the swirl number of 1.4.

**Lagrangian Velocity Comparisons** The large particle (3.5-98 \( \mu \)m) axial velocity comparisons for the two swirling cases with the data of Bonin at two different axial locations are presented in Figs. 33 (a) and (b). At the first axial location, i.e. at \( x = 0.3 \) m (Fig. 33 (a)), a swirl number of 0.8 overpredicts the particle velocity in a region near the reactor centerline. The particle velocities predicted by a swirl number of 1.4 match reasonably well with those observed experimentally. It should again be noted here that any discrepancies between the predictions and the experiments, especially in regions of reverse flow, may arise from the intrusive nature of the probe compounded with the probe's inability to measure negative velocities. For the second axial location, i.e., at \( x = 0.7 \) m (Fig. 33 (b)), both swirling cases compare reasonably with the experiments.

The results of the particle velocity comparisons indicate that marginally better predictions are obtained using the experimental swirl number of 1.4. However, considering the gas-phase results, the reduced swirl number of 0.8 appears to give better overall predictions.
Fig. 33 - Lagrangian axial velocity comparison for reacting base case using two different simulation swirl numbers (1.4 and 0.8) with experiments at (a) $x = 0.3$ m and (b) $x = 0.7$ m.
4.1.3 Concluding Remarks. The gas flow patterns show that the main features of the flow are a strong internal reverse-flow zone and an external recirculation zone. The size and strength of the internal reverse-flow zone predicted by the $k$-$\varepsilon$ model are overpredicted as compared to the experimental evidence. This leads to underprediction of the primary jet penetration. Hence, in order to artificially augment the penetration of the primary stream into the internal reverse-flow zone, the swirl number must be reduced. The reduction of the swirl number gave better predictions for the gas velocity. The predictions for the Lagrangian particle velocities did not improve by reducing the swirl number. The results presented in this study also indicate that the submodel is capable of predicting realistic estimates for the Lagrangian particle velocity magnitudes by simulating only a hundred particle trajectories. The submodel is not capable of estimating any Eulerian particle properties (such as size-resolved particle number densities) from its Lagrangian calculation, irrespective of the number of particle trajectories simulated.

4.2 Radiation Heat Transfer Modeling

The purpose of this section is to validate a radiation heat transfer model using detailed input data obtained in the CPR (Butler, 1992). The model developed in this study uses the discrete ordinates method to solve the radiative transfer equation. The sensitivity of the model predictions to those model inputs subject to uncertainty is also explored.

4.2.1 Model Description. Transport of radiant energy in a participating medium is governed by the Radiative Transfer Equation (RTE), which is written as

$$s \cdot \nabla I = - (\kappa + \sigma) I + \kappa f_b + \frac{\sigma}{4\pi} \int_0^{4\pi} \Phi(s' \rightarrow s) I' d\omega'$$

(13)

where $s$ is the unit vector in the direction of propagation. The quantities $\kappa$ and $\sigma$ are the local absorption and scattering coefficients, respectively. They depend on the absorption and scattering efficiencies and number densities of the particles, and the temperature and partial pressure of the gases. The first term in the right-hand-side represents the attenuation of intensity from absorption and scattering. The second
term is the augmentation from volumetric emission and the last term represents the augmentation due to in-scattering.

To account for separate particle and gas temperatures, Eq. (13) is modified such that two terms represent volumetric emission at the two separate temperatures as follows:

$$s \cdot \nabla I = - (\kappa_g + \kappa_p + \sigma)I + \kappa_g I_{bg} + \kappa_p I_{bp} + \frac{\sigma}{4\pi} \int \Phi(s' \rightarrow s) I' d\omega'$$  \hspace{1cm} (14)

Here, $\kappa_g$ and $\kappa_p$ are the absorption coefficients for the constituents at the gas and particle temperatures, respectively. It should be noted that at a given location in the flame the reacting particles were measured to be at different temperatures depending on size and individual reaction histories. However, the two color pyrometry measurements do not provide individual particle temperatures but a single effective temperature of the particle cloud within the measurement control volume. For the parametric study in this analysis, the single local particle cloud temperature is used to represent an average temperature. Also, because of its size, the soot was take to be at the gas temperature.

The method of solution of the RTE in axisymmetric cylindrical coordinates in this analysis is the Discrete Ordinates Method first developed for solution of the neutron transport equation (Carlson and Lathrop, 1968), and later extended to the solution of the RTE (Fiveland, 1984; Jamaluddin and Smith, 1988). The discrete ordinates method is an iterative technique for solving the RTE. Iterations proceed until a pre-selected convergence criterion is satisfied relative to changes in the local intensity. The convergence criterion used in this analysis was 0.1% change. The sensitivity to this convergence criteria was checked by comparing the prediction with this criteria with the prediction using a tighter criterion of 0.05%. The predicted wall fluxes were within a fraction of a percent each other using the two convergence criteria. After testing successively finer grids, a 40x40 grid was selected to provide adequate resolution and grid-independent predictions. Test runs were made to compare the predictions of $S_4$, $S_6$, and $S_8$ quadratures, the results of which will be discussed later. Overall radiative energy balance was demonstrated with the Discrete Ordinates RTE solver to within less than 0.1%.
4.2.2 Radiative Properties. The radiative properties of the furnace studied were calculated from the comprehensive set of field measurements which included particle number density of various size classes, percent ash in the particulates, gas and particle temperatures, CO\textsubscript{2} partial pressure, and wall temperatures. These data may be found elsewhere (Bonin, 1992; Butler, 1992; Sanderson, 1993). Linear interpolation was performed to obtain field values at grid locations. The measured values taken closest to the walls were assumed to prevail up to the wall. If the particles are approximated as spherical, homogeneous, and the complex index of refraction is known, the radiative properties of the polydispersions can be predicted using Mie theory (van de Hulst, 1957; Bohren and Huffman, 1983). Measured particle number densities were divided into eight size groups: 0.5, 1.1, 5, 10, 20, 30, 40, and 45 μm (Bonin, 1992). Both gray and spectral radiation transfer analyses were performed in this study. The determination of the spectrally-averaged properties (for the gray analyses), and the spectral properties (for the spectral analyses) is described in the following sections.

Char and Fly-Ash Spectral properties of the particulate polydispersions were calculated from Mie theory (van de Hulst, 1957; Bohren and Huffman, 1983). The Mie theory provided the spectral absorption and scattering cross-sectional areas of each size group measured. When performing gray calculations appropriate spectrally-averaged properties must be determined. If the medium is optically thin a Planck mean can be used (Siegel and Howell, 1981). Another spectral mean has been proposed by Patch which explicitly depends on optical depth (Patch, 1967). The optical thicknesses of the laboratory scale furnace studied may be classified as thin to intermediate. Gray radiative transfer predictions were performed using both Planck and Patch mean properties to investigate the differences. Comparison between the two spectral averaging techniques will be given in the next section. The spectral averaging was carried out between 1 and 18 microns which is the spectral range in which the majority of thermal radiation in coal-fired systems lies. The char radiative properties were calculated assuming a spectrally independent index of refraction of high-volatile bituminous of 1.85 - 0.22i which is representative of values reported in the literature (McCarty and Ergun, 1958; Blokh and Burak, 1973; Huntjens and van Krevelen, 1954). In those references, the index of refraction of bituminous coal was shown to depend only weakly on wavelength. The imaginary part of the index of refraction of fly-ash, on the other hand, is strongly spectrally
dependent, varying several orders of magnitude. The spectral dependence of the index of refraction of fly-ash was taken from Goodwin and Mitchner (1989). Number densities of each size group were measured without distinguishing between char and fly-ash particles. The separate number density of the char and fly-ash was approximated from the percent ash measured from particle samples taken locally (Sanderson, 1993).

The spectral division chosen for the spectral calculations was selected to accommodate the bands of the Edwards wide band model (Edwards, 1976). The spectrum was thus divided into 22 spectral bands with the radiative properties assumed uniform over each band. Solution to the Radiative Transfer Equation was carried out for each band and the resulting solutions were summed over all bands to obtain the total radiative heat transfer rates. The radiative properties of the char and fly-ash particulates summarized in the foregoing paragraphs were also used in the spectral calculations.

Due to the highly forward scattering properties of pulverized coal (Menguc and Manickavasagam, 1991), the scattering phase function was modeled with the Dirac-delta approximation as outlined by Crosbie and Davidson (1985), which is written

$$\Phi(\mu_s) = 2f\delta(1-\mu_s) + (1-f)\sum_{i=0}^{\infty} a_i P_i(\mu_s)$$

(15)

where $\delta$ is the Dirac-delta function, $f$ is the fraction of scattered radiation in the forward direction, $\mu_s$ is the cosine of the scattering angle, $P_i$ and $a_i$ are the $i^{th}$ Legendre polynomial and corresponding coefficient, respectively. The coefficients $f$ and $a_i$ were found from the original Legendre series as outlined by Crosbie and Davidson (1985). A three-term approximation for the phase function, $\Phi(\mu_s)$, was chosen since it satisfactorily models a small fraction of backscatter in addition to the forward scattering peak:

$$\Phi(\mu_s) = 2f\delta(1-\mu_s) + (1-f)[1+a_1P_1(\mu_s)+a_2P_2(\mu_s)]$$

(16)

where

$$P_1(\mu_s) = \mu_s$$

(17)

and
\[ P_2(\mu_s) = \frac{(3 \mu_s^2 - 1)}{2} \]

Fiveland has recently shown that high order quadratures of the discrete ordinates method are required for accurate integration of complex phase functions (Fiveland, 1991). In this study, it was determined that the above three-term phase function is accurately integrated with \( S_4 \) and higher quadratures by numerically integrating the above phase function over all directions.

The original Legendre coefficients were determined by trapezoidal integration of the phase function predicted by Mie theory for the polydispersion through the relation (van de Hulst, 1957)

\[ \Phi = \frac{1}{\sigma} \sum_j \sigma_j \Phi_j \]  

This was carried out for the char and fly-ash separately, from which the overall phase function coefficients were determined:

\[ b_n = \frac{1}{\sigma_{\text{char}} + \sigma_{\text{fly-ash}}} \left( \sigma_{\text{char}} b_{n,\text{char}} + \sigma_{\text{fly-ash}} b_{n,\text{fly-ash}} \right) \]  

Here, the \( b_n \)'s of each particulate constituent are the original Legendre series coefficients of the appropriate phase function. Equation (20) is similar to Eq. (19) except that the summation is over particle type (char and fly-ash) instead of size.

**Combustion Gases** The radiative properties of the combustion gases (\( \text{CO}_2 \) and \( \text{H}_2\text{O} \)) were calculated from Edwards wide band model (Edwards, 1976). \( \text{H}_2\text{O} \) concentrations were not measured since a water-cooled probe was used. No effort was made to experimentally measure the condensate from the combustion gases. Therefore, the \( \text{H}_2\text{O} \) partial pressure was estimated from the stoichiometric ratio with \( \text{CO}_2 \). The gray absorption coefficient for the gas mixture was obtained from the effective emissivity as

\[ \kappa_{\text{gas}} = -\ln(1 - \varepsilon_{\text{gas}}) / L \]
where $\varepsilon_{gas}$ is the gas emissivity and $L$ is an appropriate path length. The absorption mean beam length was used in this study (Yuen and Ma, 1992), which has been shown to be significantly different from the geometric mean beam length when scattering is present. For spectral calculations a spectral mean absorption coefficient was determined using Eq. (21) for each wide band. In regions of spectral overlap the absorption coefficient was taken as the sum of the two overlapping gaseous constituents.

**Soot** The spectrally dependent absorption coefficient for soot was taken from the relation $\kappa_\lambda = 7 f_V \lambda$ (Hottel and Sarofim, 1967), where $f_V$ is the volume fraction of the soot which has been reported in the range of $7 \times 10^{-8}$ to $4 \times 10^{-6}$ (Bard and Pagni, 1981). The baseline soot volume fraction was estimated as $3 \times 10^{-6}$ from the air and coal feed rates by assuming all the tar was converted to soot. The amount of tar is taken as 50% of the volatiles based on recent published data for the high-volatile bituminous burned in this study (Fletcher et al., 1992). The factor 7 which appears in the expression for $\kappa_\lambda$ for soot is not unique but depends on the complex index of refraction of the soot. The soot volume fraction was taken as uniform within the flame zone represented as a cone emanating from the inlet to, and extending to the walls at port 3A. The region where soot was present was determined based on $O_2$ concentration profiles in the reactor, and visual observations of the luminous region in the reactor. By contrast, the fly-ash concentrations were measured throughout the furnace (Bonin, 1992).

Wall emissivity was not measured and a baseline value of 0.8 was assumed in the predictions. The sensitivity of the radiative transfer to wall emissivity will be discussed.

### 4.2.3 Analytical Predictions

Figure 34 shows the results of one spectral and two gray calculations of the incident radiative wall flux compared with the experimental data. These predictions were obtained using $S_8$ level symmetric quadrature. All of the predictions are within 8% of the measured flux. The agreement with the measurement is good given the crude approximations of estimating the soot volume fraction and separate char and ash number densities. Accurate knowledge of the wall temperature profile and the combined char and fly-ash number density appears to be primary factors for the agreement. This is corroborated by an analytical study performed by Mengüç and Viskanta (1987), who showed that predicted radiant wall fluxes are most sensitive to the particle number density. The spectral calculation shows
Fig. 34 - Comparison of predicted incident radiative wall flux from both spectral and gray calculations with experimental data.

Fig. 35 - Measured and predicted incident wall radiant heat flux profile using $S_4$, $S_6$, and $S_8$ discrete ordinates.
the best agreement with the measured flux. The gray prediction using Planck mean properties shows better agreement with the measurement and spectral calculation than does the prediction using the Patch mean. Although the Patch mean properly accounts for thicker optical depths, the discrepancy in the Patch prediction shown is felt to be primarily due to the non-uniformity of the various field variables on which the radiative properties are dependent. The Patch mean was calculated using the local spectral absorption coefficient and an absorption mean beam length based on the entire furnace. In contrast, the Planck mean does not explicitly involve path length and is therefore defined locally. The Planck mean was chosen for the remaining gray calculations in this study.

Figure 35 shows the predicted incident radiative wall flux using level symmetric quadratures of $S_4$, $S_6$, and $S_8$ compared to the measured incident wall flux. The $S_4$ predicted flux is about 7% above the measurement at an axial distance of 30 to 40 cm. The $S_6$ and $S_8$ show better agreement in this region. Using low $S$ quadrature orders in problems of high temperature gradients can result in less accuracy due to the ray effect. $S_8$ was used in the remaining predictions discussed.

A sensitivity study was performed on the effect of the parameters which where not known, or were of significant uncertainty, on the predicted radiative incident wall flux. The uncertain parameters studied are: 1) the particle temperature, 2) the soot volume fraction, and 3) the wall emissivity. The results for the soot volume fraction are discussed below.

The effect of soot volume fraction within the flame zone is demonstrated in Fig. 36. An increase of 20% in the predicted peak incident wall flux is demonstrated when raising the volume fraction from $3 \times 10^{-7}$ to the baseline value of $3 \times 10^{-6}$. A further increase in volume fraction results in a decrease of the radiative flux at the wall adjacent to the flame zone. At these larger volume fractions self-absorption of the soot overcomes the increased local volumetric emission. The peak flux at the baseline volume fraction gives the closest agreement with the measured flux. It was found that even at the baseline volume fraction the calculated absorption coefficient of the soot within the flame was significantly higher than that associated with the particles. Soot is a primary contributor to the radiative transfer within flames of a coal furnace. This is due to the comparatively large number density of the small soot particles.
Fig. 36 - Sensitivity of predicted incident wall radiative flux to soot volume fraction.
4.2.4 Concluding Remarks. Accurate prediction of radiative transfer in pulverized coal-fired systems is critical to the determination of efficiency of combustion processes. In addition, such analyses lay the foundation for more advanced theoretical treatments of radiation/turbulence and radiation/chemistry interactions. This study illustrates the predictive accuracy of widely used RTE solver when accurate input data are available.

Predictions of the incident radiant wall heat flux compare well with the measured fluxes. The predictions indicate the importance of the role of soot on the radiative transfer within the flame. The analysis suggests the prediction techniques to be entirely adequate provided the input data are known. The analysis also suggests the general need to properly account for separate particle and gas temperatures.
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4. APPENDIX

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