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GASIFICATION IN PULVERIZED COAL FLAMES

Semi-Annual Progress Report
Department of Energy
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ABSTRACT

This project concerns the production of power and synthesis gases from pulverized coal via suspension gasification. Cyclone and confined jet gasifier configurations with swirling flow are being investigated. A unified experimental and analytical study of pulverized coal combustion and gasification in an atmospheric cyclone reactor has been performed. Experimental results include several series of coal combustion tests and a coal gasification test carried out via fuel-rich combustion. Reactor stability was excellent over a range of equivalence ratios from .67 to 2.4 and air flowrates from 25 to 100 kg/hr. Typical carbon efficiencies were 95% for air-rich and stoichiometric tests and 85% for gasification tests.

A macroscopic model for coal combustion in the cyclone has been developed. Fuel-rich gasification can also be considered through a gas-phase equilibrium treatment. Fluid mechanics are modeled by a particle force balance and a series combination of a perfectly stirred and a plug flow reactor. Kinetic treatments of coal pyrolysis, char oxidation and carbon monoxide oxidation are included. Gas composition and temperature are checked against equilibrium values. The model predicts carbon efficiency and product gas composition and temperature; gasification parameters, such as cold and hot gas efficiency and make gas heating value, are calculated for fuel-rich conditions. Good agreement exists between experiment and theory for conditions of this investigation.

Construction of the jet reactor was completed and an experimental/analytical study similar to the cyclone reactor has been initiated. A series of shakedown trials are underway and coal combustion tests will be made in the next few months.

I. OBJECTIVE AND SCOPE OF WORK

The objective of this program is to investigate the feasibility of using currently available pulverized coal burners to produce power (or synthesis) gas from coal. Two configurations are considered: (1) the annular confined jet with secondary swirl, and (2) the vortex tube with tangential entry. The first burner is characterized by a single axial injector of high primary velocity; secondary swirl is used to control mixing and residence times. The second burner is modeled after the cyclone combustor; large residence times and slagging operation should lead to high carbon efficiencies.

In both burners, coal combustion with air and/or air-oxygen mixtures supports the endothermic gasification reactions. The burners are designed such that axially injected, preheated steam is surrounded by swirling air, thus promoting efficient gasification. Pulverized coal is carried by primary steam in the confined jet system, and by primary air in the cyclone gasifier.

Species concentrations and temperature are measured both within and downstream of the gasifier chambers. These profiles are used to assess the influence of process variables such as pressure, solid/gas feed rates, swirl intensity, inlet temperature and geometrical injection pattern on both the rate and extent of coal conversion. Simple models governing entrained flow systems will be developed to further interpret the experimental data.

II. SUMMARY OF PROGRESS

The major efforts over the past ten months have been the construction of the jet reactor, and a combined experimental/analytical study of pulverized coal combustion and gasification in the cyclone reactor. A broad range of experiments has been completed in the cyclone, including early methane combustion tests, conducted to observe the reactor under clean combustion conditions. Three series of coal combustion tests and one fuel-rich gasification test (without steam addition) have also been completed. Significant results were achieved for the extended coal combustion test (series three) and the fuel-rich gasification test

(series four), including (1) an average carbon efficiency of 96% for the 46 trials of series three and (2) stable operation to an equivalence ratio of 2.4 with a carbon efficiency of 77% in series four. The best gasification results were achieved at an equivalence ratio of 2.0 where the carbon, cold gas and hot gas efficiencies were 83, 45 and 75 percent, respectively. The corresponding product gas heating value was 2.6 MJ/m^3 .

A macroscopic model for coal combustion and fuel-rich gasification in the cyclone was developed by Thomas (1978) and Barnhart (1979) to predict carbon efficiency and product gas composition and temperature. Gasification parameters, such as cold and hot gas efficiency and make gas heating value, are also calculated for fuel-rich conditions. Good agreement exists between experiment and theory for the conditions of this investigation.

Construction of the jet reactor was completed and a series of shakedown tests has been made. A hybrid-macroscopic model for the jet reactor is being developed, but no calculations have been made to date. The model uses simplified kinetics within a detailed fluid mechanics model to define the size and mass inputs to a series of macroscopic idealized reactors. Detailed homogeneous and heterogeneous kinetics are incorporated in the macroscopic portion of the model.

III. TECHNICAL PROGRESS

Facility Description

In this report, we give only a brief description of the experimental facility. A more thorough discussion may be found in Barnhart et al. (1978) and George et al. (1977).

1. Test Facility

The heart of the coal gasification facility is an explosion-proof test cell which houses the reactors, coal feeder and flow network (Fig. 1). Adjacent to the test cell is a control room from which the reactors are operated and in which a mass spectrometer plus flow and temperature monitoring stations are located. A large observation window is located between the two rooms. Support buildings not shown in Fig. 1

Figure 1. Gasification Facility Schematic

include a block structure immediately behind the test cell which houses an electric boiler and a nearby cell used for coal preparation and storage.

2. Cyclone Reactor

Table 1 lists the important features of the cyclone reactor. A vertical axis, slagging reactor was chosen to simultaneously achieve high carbon efficiency and good ash retention. Four tangential coal/air nozzles were used to make the chamber roughly axisymmetric. A chamber radius of 7.5 cm was chosen to match industrial coal throughput rates and to allow probe insertion with minimal flow disturbance.

Figure 2 is a schematic drawing of the cyclone reactor. The walls of the reactor chamber are made of Babcock and Wilcox Kaocrete refractory. The sections are held together with Satanite, a slag-resistant high alumina cement (A. P. Green Refractories Co.). A methane torch fires into the reaction chamber through the top to ignite the incoming coal/air mixture. Air and coal enter the chamber through four sets of tangential concentric stainless steel tubes. Gases leave the reactor through a throat tube which projects into the reaction chamber to prevent unreacted particles from escaping. The refractory sections are surrounded by four quarter-cylindrical heating elements (Electro-Applications, Inc.) for chamber preheat. The annular region inside the 0.6 m pressure vessel is filled with Kaowool bulk insulation (Babcock and Wilcox, Inc.).

3. Jet Reactor

Table 2 lists the major features of the jet reactor. It was designed to replicate many of the features found in industrial burners. Secondary air only is swirled via a continuously variable swirl generator. Primary air and coal are introduced at the center of the secondary air throat. The jet is fired vertically downward to minimize buoyancy-induced asymmetry and allow coal particles to settle to the exit should they become disentrained.

Figure 3 is a schematic drawing of the jet reactor. The reactor walls are 5 cm of Lightweight Castable No. 30 insulating refractory (Harbison Walker Refractories) coated on the inside with Satanite slag-resistant mortar and surrounded by 5 cm of

Table 1. Cyclone Design and Performance Characteristics

- Vertical Axis
- Slagging Reactor
- Number of Tangential Nozzles: 4
- Chamber Radius: 7.5 cm
- Length to Diameter Ratio: 1.67
- Maximum Coal Throughput: 3000 kg/hr-m³
- Heat Released at Maximum Throughput: $\sim 7.2 \times 10^7$ kJ/hr-m³

Figure 2. Cyclone Reactor Assembly

Table 2. Jet Design and Performance Characteristics

- Vertical Axis
- Downward Flow
- Concentric Fuel and Air Injection
- Variable Swirl Secondary Air
- Chamber Radius: 19 cm
- Chamber Length: 1.3 m
- Design Coal Throughput: 90 kg/hr-m³ @ 25% excess air
- Heat Release at Design Throughput: $\sim 2.3 \times 10^6$ kJ/hr-m³

Figure 3. General Layout of the Jet Reactor

packed Kaowool fiber insulation. A methane ignitor fires across the main jet about 7.5 cm downstream from the primary tube end. Gases and particulates leave the reactor through an 8.9 cm I.D. water cooled coil at the bottom of the reactor. They enter a water jacketed exhaust line immediately outside the pressure vessel. The pressure vessel is designed for operation to 20 atm.

4. Control and Monitoring System

Primary and secondary air flowrates are measured with stainless steel orifice flow meters. Product gas temperatures for each reactor are measured with a chromel-alumel thermocouple located in the center of the exhaust pipe just upstream of the cooling coil. Thermocouples are also used to monitor various reactant gas, reactor surface and gas sample temperatures. Coal is fed from a Vibra-Screw Live Bin feeder (flow range: 2-18 kg/hr; bin capacity: 50 kg) into an entrainment vessel where the pulsations induced by the feed screw are smoothed out; the pulverized coal is then carried in suspension by primary air to the reactor.

The product gas from the reactors is sampled with a stainless steel water-cooled probe located downstream of the exhaust line cooling coil. A ceramic fiber filter attached to the tip of the probe and a Balston paper filter remove particulate matter from the sample. The sampling line is heated and teflon lined (Technical Heaters, Inc.) to minimize water adsorption and catalytic reactions. A UTI Q-30C quadrupole mass spectrometer (Uthe Technology International, Inc.) with a heated inlet system is used to monitor the seven gases of interest (N_2 , O_2 , CO , CO_2 , H_2 , H_2O , CH_4). A qualitative description of the product gas is provided continuously by the mass spectrometer; quantitative analysis requires the solution of an overspecified system of linear equations (McLean and Sawyer, 1967). Details of the mass spectrometer calibration, operation and data reduction are provided by Thomas (1978).

Macroscopic Model of the Cyclone Reactor

A simple model which treats coal combustion and gasification via fuel-rich combustion for the cyclone has been developed. The model

consists of a pyrolysis zone followed by a perfectly stirred reactor (PSR) in series with a plug flow reactor (PFR). Significant features include (1) a pyrolysis model in which the volatiles yield is a function of reactor temperature and pyrolysis zone residence time; (2) a particle force balance treatment in the PSR which determines the amount of char converted to carbon monoxide (provided sufficient oxygen is present); (3) kinetically controlled conversion of CO to CO₂ in both the PSR and PFR; (4) heterogeneous char kinetics in the PFR zone and (5) a gas-phase equilibrium model which makes it possible to treat very fuel-rich cases and provides a check on the results of the kinetic analyses. The model predicts carbon efficiency, product gas composition and temperature, percent heat loss and selected gasification parameters (make gas yield, combustible make gas yield, cold and hot gas efficiency and heating value) for fuel-rich cases. We present here only the basic features of the model; details are given by Barnhart (1979) and Thomas (1978).

The combustion of coal is assumed to take place in three main steps as shown in Fig. 4. The regions within the cyclone corresponding to the three steps are illustrated in Fig. 5. The major governing assumptions for each zone are given in Table 3. The model can be arranged to treat two basic cases: (1) an isothermal case in which the temperature of the entire cyclone is an input parameter and (2) a nonisothermal case in which all reactor heat losses are assumed to come from the PSR zone and energy conservation is used to calculate the PSR and PFR zone temperatures. The reactor heat losses predicted by the heat transfer analysis are about 10% less than those observed experimentally, resulting in unreasonably high reactor temperatures. Thus the isothermal version of the model is currently used for comparison with experimental results and is described herein; the full details of the nonisothermal version are presented by Thomas (1978). Future work will consider a more sophisticated heat transfer model.

1. Pyrolysis Zone

Incoming coal particles are assumed to follow a Rosin-Rammler size distribution as recommended by Field et al. (1967). The incoming coal-air mixture enters the pyrolysis zone at high velocity; due to

Figure 4. Cyclone Combustor Model Schematic

Figure 5. Hypothesized Cyclone Reaction Zones

Table 3. Cyclone Model Assumptions

Pyrolysis Zone

1. Input coal particles follow a Rosin-Rammler size distribution.
2. Gas temperature in the pyrolysis zone is constant and equal to the PSR zone temperature. Particle temperature is determined by a simple radiation-convection heat transfer model based on the mass average particle diameter.
3. The particle residence time is a factor of ten greater than the gas residence time. The rate and extent of devolatilization are determined by the kinetic weight loss model of Kobayashi et al. (1977).
4. All of the coal H, N, O and S is lost in pyrolysis; all ash is retained in the char.
5. Volatiles burn instantaneously to form H_2O , NO , SO_2 and CO ; no CO_2 is produced.
6. Particles swell in diameter by 10%.

PSR Zone

1. Particles entering the PSR zone, whose size is greater than a critical size, burn forming CO as the only product until reaching the critical size (provided adequate oxygen is present to convert all the released carbon to CO). These particles are then passed on to the PFR zone at this critical size, which is determined from a particle force balance. Particles which enter the PSR zone whose diameter is smaller than the critical particle size are completely burned before reaching the PFR.
2. When insufficient oxygen is present, particles burn only until the available oxygen is depleted. Product gas composition is then determined by an equilibrium analysis.
3. The char ash is lost at a rate proportional to carbon combustion, such that the char composition remains constant throughout the reactor.
4. Homogeneous conversion of CO to CO_2 (and corresponding O_2 depletion) is calculated assuming the zone to be a micromixed perfectly stirred reactor.
5. All heat losses from the reactor occur in the PSR zone.

Table 3. (cont.)

PSR Zone (cont.)

6. The kinetically determined CO-CO₂ conversion is checked against the limitations imposed by gas-phase equilibrium.

PFR Zone

1. The input particles are monosize and equal to the critical diameter determined by the PSR force balance treatment.
2. Reactants enter the PFR zone in an evenly distributed fashion along the entire length of the zone which is not enclosed by the throat tube.
3. The PFR zone is adiabatic for the nonisothermal case and isothermal for the constant temperature case.
4. The kinetically determined CO-CO₂ conversion is checked against the limitations imposed by gas-phase equilibrium.

intense convective heating from the chamber walls and to intimate mixing with hot gases, the air is rapidly heated and is thus assumed to reach the PSR zone temperature instantaneously. Particle temperatures are assumed to lag behind the gas temperature and are calculated on the basis of a simple heat transfer model which includes convection from the surrounding gases and radiation from the flame and chamber walls (Barnhart, 1979). The resulting expression for particle heating rate is integrated numerically to yield particle temperature as a function of time. The observed particle heating rates are on the order of 10^5 to 10^6 °K/sec and are comparable to values cited in the pyrolysis literature (Kimber and Gray, 1967; Kobayashi et al., 1977).

The particle temperature history is used in conjunction with the pyrolysis model of Kobayashi et al. (1977) to predict volatiles yield as a function of time. The Kobayashi model is applicable to the full range of temperatures encountered in the cyclone and is readily implemented once corrections are made to consider moisture-containing coals. In this model, two competing overall reactions are considered which together provide a better correlation with experimental data than is possible with a single-reaction model. The coal mass fraction volatilized is given by

$$f_v = \int_0^t (\alpha_1 k_1 + \alpha_2 k_2) \exp\left[-\int_0^t (k_1 + k_2) dt\right] dt, \quad (1)$$

$$k_1 = B_1 \exp(-E_1/RT_p) \quad (2)$$

$$k_2 = B_2 \exp(-E_2/RT_p) \quad (3)$$

where α_1 and α_2 are mass stoichiometric coefficients (as-received basis), B_1 and B_2 frequency factors (sec^{-1}), E_1 and E_2 activation energies (kJ/gmole), R is the universal gas constant (kJ/gmole-K) and T_p the particle temperature (K). The mass stoichiometric coefficients α_1 and α_2 correspond to the maximum yields at infinite time for the low and high temperature mechanisms, respectively; moisture is assumed to be evolved at low temperatures (Solomon, 1977).

A closed form solution to Eqn. 1 can be obtained by assuming a constant particle temperature; yields are thus calculated in a step-wise isothermal fashion. The resulting volatiles mass fraction is a strong function of gas temperature, ranging from 6% at 1100K to 50% at 2000K. The particle weight loss with time, when converted to a dry ash-free basis, agrees closely with the theoretical curves of Kobayashi et al. (1977) for the full range of temperatures considered.

For moderate gas temperatures (<1500K, typical of gasification conditions) coal particles require 150 msec or more to pyrolyze. Gas residence times in the pyrolysis zone range from 4 to 20 msec; however, particle residence times are assumed to be an order of magnitude larger based on the findings of Lewellen et al. (1977) and Agrest (1965). For gas temperatures of ~1500K, the pyrolysis yield is then limited by particle residence time for air flowrates of 50 kg/hr and greater. This is particularly significant under gasification conditions since carbon efficiency and CO + H₂ yield are enhanced by high air flowrates (Barnhart, 1979).

All of the coal H, N, O, S and moisture are assumed to devolatilize, even in those cases (low temperature and high air flowrates) when the predicted volatiles mass fraction is less than the combined mass fractions of the above constituents; thus the char particle is simply ash and carbon. Volatiles burn instantaneously forming H₂O, NO, SO₂ and CO. Following Essenhigh (1977), a 10% increase in particle diameter is assumed to account for coal swelling. The flowrates of char and gaseous species leaving the pyrolysis zone are calculated with simple conservation equations based on the coal ultimate analysis, the incoming coal and air flowrates and the coal mass fraction volatilized.

2. PSR Zone

a. Particle behavior and homogeneous kinetics

A PSR was chosen to model the majority of the reaction chamber due to the large recirculation zones and high turbulence levels present in cyclones. In perfectly stirred reactor theory mixing occurs at an infinite rate and the mixture properties (temperature and species concentrations) are equal to those of the exiting stream. Thus a detailed

description of the fluid and particle mechanics (an impossible task at present) is not required. The important features of the PSR analysis are char and CO oxidation and an external heat transfer model for the nonisothermal analysis.

The extent of char oxidation to CO in the PSR zone is determined by a particle force balance adapted from Perry et al. (1950). The force balance includes the viscous drag of the gases and the swirl-induced centrifugal force, yielding the following expression for the radius a of a particle in equilibrium at the cyclone throat radius R_t (Thomas, 1978):

$$a = \frac{3}{2} P_f (L - L_t) (R - R_t) \frac{R_t}{R} (\mu / \pi \rho \dot{V} L)^{1/2} \quad (4)$$

where L and L_t are the chamber and throat tube lengths, R and R_t are the chamber and throat tube radii, μ is the gas viscosity, ρ the particle density, and $\dot{V}$ the volumetric flowrate. Owing to the large particle residence time in the PSR, a char particle oxidizes until its radius equals a , at which point it enters the PFR zone. Ash accumulates in the form of slag at the same rate carbon is burning so particle composition remains constant. The particle force balance parameter P_f is a correction factor which is adjusted to create agreement between the calculated particle radius and values obtained experimentally in a Plexiglas model of the cyclone (Thomas, 1978); a value of $P_f = 2$ is satisfactory. Particles entering the PSR with radii less than a are completely converted to CO in the PSR.

As a result of the force balance treatment, the rate of char oxidation in the PSR can be calculated from a simple mass balance of particles entering and leaving the PSR zone (Thomas, 1978). Another consequence of this treatment is that the particles entering the PFR are monosize with a radius equal to the critical radius a .

The homogeneous combustion of carbon monoxide is modeled using the overall Arrhenius expression of Howard et al. (1973):

$$r_{CO} = k_0 [CO] [O_2]^{1/2} [H_2O]^{1/2} \exp(-E/RT) \quad (5)$$

where k_0 is the pre-exponential factor, $[CO]$, $[O_2]$ and $[H_2O]$ are gas concentrations (kgmole/m^3), E is the activation energy (kJ/gmole) and T the temperature (K). The flowrate of CO leaving the PSR, $F_{CO,o}$ (kgmole/hr), can be calculated by species conservation:

$$F_{CO,o} = F_{CO,i} + r_C V_{PSR} - r_{CO} V_{PSR} \quad (6)$$

where $F_{CO,i}$ is the CO flowrate into the PSR zone, $r_C V_{PSR}$ is the rate of char oxidation to CO and $r_{CO} V_{PSR}$ is the rate of conversion of CO to CO_2 (kgmole/hr). The flowrates of other gaseous species leaving the PSR zone are calculated via simple mass balances (Thomas, 1978).

b. Stoichiometric limitations

The analysis cannot proceed as indicated in Eqn. 6 if insufficient oxygen exists to convert all the char carbon released in the PSR to CO ; this occurs when $2F_{O_2,i} < r_C V_{PSR}$ where $F_{O_2,i}$ is the oxygen flowrate into the PSR zone (kgmole/hr). For the coals used in this investigation (see Table 6) this limitation corresponds to an air/coal ratio of approximately 55% of stoichiometric. For air/coal ratios below this point, the char oxidation rate is calculated as

$$r_C V_{PSR} = 2F_{O_2,i} \quad (7)$$

The outlet flowrates of CO , CO_2 , H_2 , H_2O and O_2 are then determined through C , H and O balances and two chemical equilibria: (1) $CO_2 \rightleftharpoons CO + \frac{1}{2}O_2$ and (2) $CO_2 + H_2 \rightleftharpoons CO + H_2O$.

To summarize, the amount of char carbon converted to CO is determined by either the force balance treatment or the amount of available oxygen. In the former case the amount of CO_2 formed is determined by kinetics (Eqn. 5) and all hydrogen remains in the form of H_2O ; in the latter case, the PSR gas composition is determined by chemical equilibrium.

c. PSR equilibrium checks

The results of the kinetically controlled conversion of CO to CO₂ are checked against the limitations imposed by equilibrium to prevent second law violations. A direct comparison is made between the kinetic and equilibrium CO/CO₂ ratios. Second law violations occur relatively frequently, especially for fuel-rich cases above 1500K, but the effect of reverting to equilibrium values on gross behavior is negligible.

When oxygen is depleted in the PSR during fuel-rich runs, the conversion of CO to CO₂ is halted and the species flowrates are "frozen" at that point. This situation is not realistic because other mechanisms are available to carry this system toward equilibrium. To remedy this situation, the gas-phase constituents are assumed to go to equilibrium. Results of Elliott et al. (1952) and the present investigation show that the gas-phase composition is reasonably close to equilibrium for the fuel-rich cases.

3. PFR Zone

A plug flow reactor was chosen for the exit region because of the lower levels of turbulence and the resemblance to pipe flow. The gases and monosize char particles leaving the PSR zone are evenly distributed into the PFR zone over the entire PFR length except for that portion enclosed by the throat tube (Fig. 5). Reactions continue until the reactants reach the cooled portion of the cyclone exhaust where they are quenched. The PFR zone is broken up into roughly 300 discrete increments to insure calculation accuracy.

The rate of carbon monoxide oxidation within each increment of the PFR zone is calculated via Eqn. 5. The concentrations required for this expression are based on the incoming molar flowrates. The oxidation of char in the PFR zone takes place under combined kinetic and diffusion control, expressed as (Laurendeau, 1978)

$$R_e = [O_2]_0 / (1/K_D + 1/K_C) \quad (8)$$

where R_e is the reaction rate based on external surface area ($\text{kg/m}^2\text{-s}$), $[O_2]_0$ the bulk concentration of oxygen (kg/m^3), K_D the rate of oxygen diffusion to the particle surface (m/s) and K_C the chemical reaction rate coefficient at the surface (m/s).

For particles under $100\ \mu\text{m}$, K_D can be calculated assuming a stagnant gas film around a spherical char particle (Laurendeau, 1978); hence,

$$K_D = 2 \Lambda D/d \quad (9)$$

where Λ is the gravimetric stoichiometric coefficient (kg-C/kg-O_2), D the molecular diffusivity for oxygen (m^2/s) and d the particle diameter (m). K_C is expressed by the Arrhenius expression

$$K_C = A \exp(-E/RT) \quad (10)$$

where A is the pre-exponential factor, E , R and T are as previously defined. For pulverized bituminous char, Smith (1971) found E and A to be $67\ \text{kJ/mole}$ and $80\ \text{kg/m}^2\text{-s-atm}$, respectively for $1200 < T < 2270\text{K}$.

The char and gaseous species flowrates leaving an increment are calculated with simple species conservation equations (Thomas, 1978). The results of the kinetic analysis are checked against equilibrium results in exactly the same fashion as in the PSR zone. The calculation of carbon efficiency (and gasification parameters for fuel-rich runs) at the end of the PFR is straightforward, as demonstrated by Barnhart (1979).

4. Model Characteristics

The model makes no attempt to describe in detail the actual particle behavior and fluid mechanics in the cyclone; simple concepts are used instead to better understand overall reactor performance. Different model components have a dominant influence on reactor behavior for various ranges of stoichiometry. For very fuel-rich cases the carbon efficiency is controlled by oxygen depletion in the PSR and product gas composition is determined via the equilibrium treatment. For moderately fuel-rich and stoichiometric cases the PSR force balance treatment dominates and

for air-rich cases (particularly at high temperature) the oxidation of char in the PFR zone becomes important. The model is superior to a simple equilibrium treatment or a pure PSR because of its ability to treat a wide range of experimental conditions. Model parameters used for comparison to the experimental results of the next section are given in Table 4.

Experimental Results and Comparison with Cyclone Reactor Model

A broad range of experiments has been completed in the cyclone, including two series of methane combustion tests, conducted to observe the reactor under clean combustion conditions. Three series of coal combustion tests and one fuel-rich gasification test have also been completed. The important results of the methane tests and the early coal tests will be presented only briefly. Emphasis is on the extended coal combustion test (series three) and the fuel-rich gasification test (series four) in which truly significant results were achieved, including (1) an average carbon efficiency of 96% for the 46 trials of series three and (2) stable operation to an equivalence ratio of 2.4 with a carbon efficiency of 77% in series four. The experimental data of series three and four are tabulated in detail in Barnhart (1979).

1. Data Reduction

A computer program is used to analyze the raw experimental data and to calculate exhaust gas concentrations and temperature, gas flow-rates, reactor heat loss, performance parameters and mass balance errors. The total product gas flowrate is calculated using nitrogen as an inert tracer. Due to difficulties in sampling for water vapor, the data reduction procedure presently uses the original spectrum on a dry basis and then adds enough water vapor to create a perfect oxygen balance. Carbon efficiency is unaffected since only the water vapor molar flowrate is altered. However, sensitivity studies using typical hydrogen and oxygen mass balance errors generated by the original data indicate that the carbon efficiency is accurate to $\pm 5\%$. The average hydrogen mass balance error for the 67 trials of series 3 and 4 was 8.9%, and in 75% of the cases the error was under 12%. Typical total mass balance errors are

Table 4. Parameter Values Used for Model Calculations

<u>Quantity</u>	<u>Symbol</u>	<u>Value</u>
Cyclone Geometry		
Chamber Length	L	.25 m
Chamber Radius	R	7.5 cm
Throat Tube Length	L_t	5.0 cm
Throat Tube Radius	R_t	2.0 cm
Throat Tube Length Plus Uncooled Portion of Exhaust	ℓ_t	.165 m
Coal Properties		
Density	ρ	1360 kg/m ³
Specific Heat	c_p	1.26 kJ/kg-K
Average Particle Diameter	d_p	53 μ m
Rosin-Rammler Dispersion Index	x	1.2
Particle Emissivity	ϵ_p	1.
Pyrolysis Parameters		
Swelling Index	s	1.1
Mass Stoichiometric Coefficients	α_1	.3
Frequency Factors	α_2	1.
	B_1^2	$2 \times 10^5 \text{ s}^{-1}$
Activation Energies	B_2^2	$1.3 \times 10^7 \text{ s}^{-1}$
	E_1	105 kJ/gmole
	E_2	168 kJ/gmole
Carbon Monoxide Kinetics		
Frequency Factor	k_0	$1.3 \times 10^{11} \text{ m}^3/\text{kgmole-s}$
Activation Energy	E_0	126 kJ/gmole
Char Kinetics		
Frequency Factor	A	$80 \text{ kg/m}^2\text{-s-atm}^\dagger$
Activation Energy	E	67 kJ/gmole

[†]1 atm = 101.3 kPa

1-3%. Full details of the data reduction procedure are presented by Barnhart (1979).

2. Methane Combustion Tests

Preliminary tests introduced methane to the cyclone via the torch ignitor. The resulting fires proved to be clean and extremely stable and were thus well suited for preliminary measurements under "steady state" conditions. The early methane tests were conducted primarily to confirm the reliability of the product gas sampling system (Thomas, 1978; Barnhart, 1979). More recently, methane flames were used to provide cyclone exhaust temperature and species profiles. A velocity traverse was also conducted but under cold flow conditions. The species profile was flat as expected; the temperature and velocity profiles were influenced by the exhaust cooling coil (Fig. 2) and swirl-induced axial recirculation. Reverse flow occurred in the central 3 cm of the exhaust pipe, resulting in a fairly substantial exhaust thermocouple radiation correction of 100 to 200K (Barnhart, 1979).

3. Coal Combustion Tests

A summary of all cyclone coal combustion tests is presented in Table 5. Analyses of the three coals used in the experiments (performed by Commercial Testing and Engineering Co.) are presented in Table 6. In all four series of tests a trial or data point is based on one set of flow and temperature data and the average of two mass spectra taken concurrently.

a. Series one

Early coal combustion tests were characterized by low exhaust temperatures ($<1250\text{K}$) that fluctuated as much as 200K in a matter of minutes. The average carbon efficiency was 95%; however, values ranged from 78 to 113% and hydrogen mass balances were poor. Slagging conditions were achieved but the behavior of the slag was not satisfactory. The slag port quickly bridged over and slag eventually accumulated to a depth of 2 cm in the bottom of the reactor. Molten slag was entrained by the exiting gases and deposited on the throat tube, nearly closing

Table 5. Coal Combustion Test Summary

<u>Series</u>	<u>Trials</u>	<u>Coal Type</u>	<u>Stoichiometry[†]</u> <u>(A/F)/(A/F)_S</u>	<u>Air Flow</u> <u>(kg/hr)</u>	<u>Coal Feed Rate</u> <u>(kg/hr)</u>
1	15	Indiana Bituminous	1.20-1.75	45-80	3.3-7.3
2	8	Montana Subbituminous	1.20-1.40	40-70	4.3-6.8
3	46	Montana Subbituminous	.820-1.50	25-100	4.5-9.0
4	21	Montana Subbituminous	.420-1.30	35-60	4.5-14

(A/F)/(A/F)_{STOICH} is the reciprocal of the equivalence ratio; its use here corresponds to accepted practice in the coal combustion and gasification literature.

Table 6. Coal Analyses

	<u>Indiana Bituminous</u>		<u>Rosebud Seam Subbituminous</u>		<u>McKay Seam Subbituminous</u>	
Proximate Analysis (%)	<u>As Rec'd</u>	<u>Dry Basis</u>	<u>As Rec'd</u>	<u>Dry Basis</u>	<u>As Rec'd</u>	<u>Dry Basis</u>
Moisture	15.33	XXXXX	13.99	XXXXX	13.70	XXXXX
Ash	14.67	17.33	10.02	11.65	11.24	13.02
Volatile	32.61	38.51	33.31	38.73	31.31	36.28
Fixed Carbon	37.39	44.16	42.68	49.62	43.75	50.70
Heating Value (kJ/kg)	23400	27600	23000	26700	22600	26200
Ultimate Analysis (%)						
Moisture	15.33	XXXXX	13.99	XXXXX	13.70	XXXXX
Carbon	55.54	65.60	58.54	68.06	57.35	66.46
Hydrogen	4.00	4.73	3.79	4.41	3.63	4.21
Nitrogen	1.07	1.26	0.82	0.95	1.01	1.17
Chlorine	0.02	0.02	0.01	0.01	0.03	0.03
Sulfur	2.88	3.40	0.93	1.08	1.41	1.63
Ash	14.67	17.33	10.02	11.65	11.24	13.02
Oxygen	6.49	7.66	11.90	13.84	11.63	13.48
Ash Fusion Temp. (K)	<u>Reducing</u>	<u>Oxidizing</u>	<u>Reducing</u>	<u>Oxidizing</u>	<u>Reducing</u>	<u>Oxidizing</u>
Initial Deformation	1405	1465	1405	1485	1405	1490
Fluid	1500	1590	1465	1565	1470	1565

it and forcing an end to the tests. Thus the behavior of the cyclone in terms of stability and operability left much to be desired.

b. Series two

A Montana subbituminous coal from the Rosebud seam was used in series two because of its slightly lower ash fusion temperature (Table 6). Slag flow was only marginally improved, and slag deposition in the throat tube once again forced a premature end to the series. The average carbon efficiency was high (96%) and reactor stability was much improved. The internal consistency of the data was also good with an average hydrogen mass balance error of 12.6%. Thus, with the exception of the slagging problem series two represented a significant improvement over series one.

c. Series three

A mixture of equal parts by weight of Rosebud and McKay seam coals was used in series three to improve slag flow; the ash fusion temperature of such a mixture is $\sim 35\text{K}$ lower than that of either of the two burned alone (Barnhart, 1979). Although the slag port bridged shut again, the rate of accumulation of slag in the throat tube was much lower. The throat tube was cleared after six trials were completed and testing then proceeded uninterrupted for six hours.

In Fig. 6 carbon efficiency is plotted as a function of stoichiometry for three ranges of air flowrate. Any effect of stoichiometry or air flowrate on carbon efficiency is masked by the scatter in the data. The average carbon efficiency (96%) and hydrogen mass balance error (6.8%) for this series are both very good.

Also plotted on Fig. 6 are the carbon efficiencies predicted by the cyclone model for air flowrates of 35, 60 and 85 kg/hr and a reactor temperature of 1800K -- the average experimental exhaust temperature. Theoretical carbon efficiencies increase with air flowrate due to enhanced centrifugal effects in the PSR zone which decrease the radius of particles entering the PFR zone (Eqn. 4). Increased air/fuel ratio increases carbon efficiency due to the linear dependence of char

Figure 6. Series Three Experimental and Theoretical Carbon Efficiencies as Functions of Normalized Air/Fuel Ratio. The slashed (/) data points indicate the first six trials.

oxidation rate on oxygen concentration in the PFR zone (Eqn. 8). The effect in both cases is minimal. Thus the range of values predicted by the model and the effects of air flowrate and stoichiometry are in close agreement with the experimental results for the conditions of series three.

d. Series four.

The object of the fourth series of coal tests was to gasify coal without steam addition by proceeding systematically to lower air fuel ratios. A mixture of Rosebud and McKay subbituminous coals was once again used. The reactor configuration was altered somewhat during the test by a mechanical failure which went unnoticed until the post-test inspection; however, the effect on the experimental results is believed to be small for reasons to be discussed later.

The experimental carbon efficiencies are plotted versus stoichiometry for two air flowrate ranges in Fig. 7. The trials on the air-rich side were performed under very carefully controlled conditions as a test of repeatability; the results are satisfactory. The carbon efficiency is high (above 90%) down to about 55% of stoichiometric air at which point a smooth but steep decrease begins. The solid curve in Fig. 7 represents the carbon efficiencies predicted by the model for the conditions of the experiment (1800K for air-rich cases; 1600K for fuel-rich). The agreement with the experimental data is very good, although the model predictions at very low air/fuel ratios are somewhat low. The effect of air flowrate is again minimal.

Interpretation of the observed experimental results in terms of the model assumptions is straightforward. The particle force balance treatment, which dictates the amount of carbon burned in the PSR, is the dominant factor for stoichiometries above $(A/F)/(A/F)_S = .55$. For stoichiometries below this point the amount of oxygen in the PSR is insufficient to convert all the char carbon to CO; this limitation overrides the force balance treatment and thus more unburned carbon leaves the reactor as the air/fuel ratio is reduced. Steam and carbon dioxide oxidation of the char were not included in the model because they proceed at a much lower rate than that of char oxidation by oxygen (Laurendeau,

Figure 7. Series Four Experimental and Theoretical Carbon Efficiencies as Functions of Normalized Air/Fuel Ratio.

1978); the results at very low air/fuel ratios might well improve, however, if these mechanisms are included in future modifications.

The results of series four were also analyzed in terms of commonly used gasification performance indicators (George et al., 1977); the three most important parameters are plotted in Fig. 8 as functions of air/coal ratio. The experimentally determined product gas heating values increase almost linearly with decreasing air/fuel ratio to a peak value of 3.1 MJ/m^3 . Heating values predicted by the model are only slightly higher than those found experimentally for air/coal ratios above 4.0; however, below this point the theoretical heating values decrease sharply while the experimental values continue to increase.

Heating value is directly proportional to the sum of the product gas CO and H_2 mole fractions since their heats of combustion are nearly identical and no methane was produced. The theoretical and experimental $(\text{CO} + \text{H}_2)$ yields (m^3/kg coal) are in close agreement for values of air/coal down to 4.0; at this point the theoretical values begin to decrease because of the sharp decrease in theoretical carbon efficiency (Fig. 7). The experimental $(\text{CO} + \text{H}_2)$ yield however, continues to increase; such a trend at low air/coal ratios is indicative of char oxidation by steam:

Thus it appears that the omission of this mechanism in the model is responsible for the incorrect trend in make gas heating value, as well as the low carbon efficiencies observed in Fig. 7.

Also plotted on Fig. 8 is the cold gas efficiency, defined to be that portion of the coal heating value present as chemical enthalpy in the product gas. The cold gas efficiency is proportional to the product of the make gas heating value and the make gas yield (kg make gas/ kg coal), neglecting the change in product gas molecular weight with air/coal ratio (Barnhart, 1979). Make gas yield was found to increase linearly with air/coal ratio both experimentally and theoretically; thus one would expect the ratio of cold gas efficiency to make gas heating

Figure 8. Hot Gas Efficiency, Cold Gas Efficiency and Heating Value Versus Air/Coal Ratio. The stoichiometric air/coal ratio is 7.5.

value to increase linearly with air/coal ratio, a trend that both the experimental data and model predictions follow.

The third parameter plotted on Fig. 8 is the hot gas efficiency, which includes the change in sensible enthalpy between reactants and products as well as the change in chemical enthalpy and is expressed as (Laurendeau and Waite, 1977):

$$\eta_{hg} = \eta_{cg} + \Delta H_{pr} / \Delta H_{C,coal} \quad (12)$$

where η_{hg} and η_{cg} are the hot and cold gas efficiencies, ΔH_{pr} is the difference in sensible enthalpy between reactants and products (kJ/kg coal) and $\Delta H_{C,coal}$ is the coal heat of combustion (kJ/kg coal). The hot gas efficiency is a significant performance indicator when the sensible enthalpy of the product gas can be used directly for process heat. Note that η_{hg} equals η_{cg} plus a term which is a strong linearly increasing function of both temperature and air/coal ratio. The influence of the second term is especially clear for the theoretical curves which are based on the isothermal model at a constant temperature of 1600K; the difference between the hot and cold gas efficiencies increases steadily with air/coal ratio. The scatter in the experimental hot gas efficiency values is due to cases in which the reactor temperature was substantially different from the average value of 1600K; most noticeable is the point at air/coal = 6.4 for which the exit temperature was 1860K. With the exception of this point, the comparison between experimental and theoretical hot gas efficiencies is very similar to that between experimental and theoretical cold gas efficiencies as would be expected.

A further check on the consistency of the experimental data was made by comparing the experimentally determined value of the water-gas shift equilibrium constant (based on the observed mole fractions) to the value based on the exit temperature (Fig. 9). The experimental values are in reasonably close agreement with the theoretical curve, especially considering the short gas residence time in the cyclone (~50 msec) and the uncertainties in measuring mole fractions and temperatures.

Figure 9. Experimental and Theoretical Values of the Water-Gas Equilibrium Constant

Inspection of the cyclone after completion of series four revealed that at some time during the test the exhaust throat tube (Fig. 2) broke loose from the top of the chamber and fell into it, blocking the exhaust port. The gases then left the reactor through a narrow gap which opened up between the top two refractory sections. Under most conditions, the effect of this change in configuration on reactor performance would more than likely be detrimental, since unreacted particles would probably escape with the gases. However, under the strongly fuel-rich conditions of this test, the carbon efficiency should be determined by oxygen depletion and the exhaust composition by water-gas equilibrium. Since the oxygen level in the product gas was negligible and the product gas was indeed very close to water-gas equilibrium (Fig. 9), the effect on reactor performance was apparently minimal.

4. Comparison with Literature Results

The only substantial results available for gasification via fuel-rich combustion in a cyclone reactor are reported by Traenckner (1953) for the Ruhrgas process. A gas with a heating value of 3.7 MJ/m^3 was produced at an equivalence ratio of 2.0; however, the carbon efficiency was increased from 80 to 95% through particle recycle. Without particle recycle the heating value would be expected to decrease; if the decrease in heating value is roughly proportional to the decrease in carbon efficiency, the resulting heating value would be very similar to the maximum value achieved in the present investigation (3.1 MJ/m^3). Note also that the data reported by Traenckner was at an equivalence ratio of 2.0, the optimum operating point for the present investigation based on trends in heating value and carbon, cold gas and hot gas efficiencies (Figs. 7 and 8).

Perry et al. (1950) compare experimental and theoretical values of the water-gas shift equilibrium constant for a steam/oxygen cyclone gasifier as was done in Fig. 9; their correlation shows similar agreement. They also report a nearly linear decrease in carbon efficiency with decreasing oxidizer/coal ratio for typical gasification stoichiometries; the same trend is evident in the present investigation (Fig. 7) and in the results of two non-swirling entrained flow studies reviewed by

Lenzer (1977). The scatter in the experimental carbon efficiencies of this investigation (Figs. 6 and 7) is comparable to that reported by Elliott et al. (1952).

In summary, comparison with the available literature is difficult because of the scarcity of data and the different conditions under which various systems were operated. In spite of this, however, it appears that the results achieved during this investigation show satisfactory agreement with the results of previous researchers.

Jet Reactor Shakedown Runs

A series of tests was conducted on the jet reactor with methane combustion only to identify possible problem areas before coal operations were begun. The methane torch is quite easy to light off and remains stable over a very large range of flowrates and overall stoichiometries owing to the relatively low transverse velocities at the torch exit. Refractory temperatures in excess of 900°K were achieved.

Following the reactor tests, a thorough inspection of the reactor internals was made. No problems were noted beyond a few hair-line cracks in the Satanite mortar at refractory joints.

The shakedown run did, however, identify three operational problems. It was found that virtually all the water generated as a result of combustion condensed either on the cooling coil or in the exhaust line and collected at the clean-out cap at the bottom of the reactor. Sufficient water was collected during a 1-1/2 hour run to inundate the probe so that liquid water was pulled into the mass spectrometer. Light fuel oil used to clean the parting agent from the refractory baked out of the refractory and was also pulled into the mass spectrometer. A complete cleaning of the mass spectrometer was required. To circumvent this problem, a longer probe which reaches beyond the highest possible water level was been fabricated and a conductivity alarm will be installed on the mass spectrometer inlet. During coal runs, water collection should be greatly reduced due to higher temperatures and lower hydrogen content.

a. Relative location of subreactors

b. Subreactor flow schematic

Figure 10. Jet Reactor Layout

The primary tube was observed to be glowing brightly as a result of heating by the central recirculation zone. In order to prevent oxidation of the tube, the run procedure has been modified to include a small flow of primary air at all times. Overheating the primary pipe has clearly demonstrated the existence of a central recirculation zone which extends into the burner throat.

Nitrogen consumption to cool the sight glass and the surrounding pressure vessel was excessive, and provisions were made for diverting a small portion of the secondary air flow through the cooling ports. Even with increased cooling, this portion of the shell reached 400°K compared to 330°K for the cooler portions. The temperature differential did appear to be stabilizing, however, and since the vessel is designed for 600°K , no action will be taken other than close monitoring during initial coal runs.

A second series of methane combustion tests followed by coal combustion tests will be initiated upon recalibration of the mass spectrometer. The next series of methane tests is designed to demonstrate the ability of the sampling system and mass spectrometer to give accurate water readings even under high moisture content conditions.

Jet Reactor Model

The macroscopic reactor series model has proven quite effective for the cyclone. The allocation of reactor volumes in the jet is less straightforward since the fluid mechanics are strongly influenced by swirl, nozzle shape, and confinement ratio (George, 1978). In order to provide a basis for the assignment of subreactors, a hybrid modeling approach is being pursued. A finite difference solution to the governing equations for two dimensional recirculating elliptical flow with a $k-\epsilon$ turbulence model and simple chemical kinetics will be used to identify size and mass flow through various subreactors. This modeling approach was selected since it is general enough to be widely used both for prediction and correlation, but the computational requirements are moderate (Swithenbank et al., 1978). A fluid mechanics computer program now being used by Professor D. B. Spalding at Purdue

can be adapted to the jet reactor problem and will greatly reduce the model development time (Spalding, 1978).

The fluid mechanics model will provide a map of streamlines and turbulence kinetic energy distributions. Regions with closed streamlines will be characterized as stirred tank reactors with other areas being designated as plug flow reactors.

Figure 10 shows the expected subreactor arrangement and dominant kinetic paths. Since fluid crosses streamlines by diffusion only, reactor mass interchange will be based on exchange coefficients developed from the kinetic energy of turbulence and an approximate concentration gradient at the reactor boundaries. Coal particle slip will be incorporated by using exchange coefficients modified by the Stokes number of the particles following Yuu et al. (1978). The fluid crossing the boundary is typical of the local fluid composition of the source reactor. Hence, all fluid leaving the PSR's is of a single composition while fluid leaving the PFR's varies with axial location. With boundaries and mass fluxes defined, detailed kinetic schemes can be included in the subreactor models to account for Langmuir-Hinshelwood char kinetics with O_2 , H_2O and CO_2 , product dissociation and pollutant formation (Finson et al., 1978).

IV. WORK FORECAST

Before the end of the contract, we expect to accomplish the following:

- (1) obtain combustion and fuel-rich gasification data for the jet reactor at 1 atm
- (2) develop a hybrid model for the jet reactor
- (3) analyze fuel-rich gasification at higher throughputs in the cyclone reactor (time and funds permitting).

V. RESULTS AND CONCLUSIONS

A unified experimental/analytical approach to pulverized coal combustion and gasification in a cyclone reactor has been developed.

The emphasis in the experimental portion of this work was directed toward coal combustion and gasification via fuel-rich combustion with air at atmospheric pressure. Carbon efficiencies during coal combustion tests were excellent (90 to 100%) and were largely insensitive to changes in air flowrate and air/fuel ratio. Under gasification conditions the best results were achieved at an equivalence ratio of 2.0 where a gas with a heating value of 2.6 MJ/m^3 was produced. The corresponding carbon, cold gas and hot gas efficiencies were 83, 45 and 75%, respectively,

Slag accumulation was a problem throughout the tests. Although reducing the time available for experimental runs, the slag problem had no apparent effect on the nature of the experimental results. The operability of somewhat larger cyclones under slagging conditions has been amply demonstrated (Elliott et al., 1952; Joubert, 1978); thus achieving successful slag flow need not be a primary concern in this investigation.

Future cyclone experiments should be directed toward gasification via (a) fuel-rich combustion and (b) moderate steam addition. Internal sampling should be used to facilitate more detailed comparisons with model predictions, particularly at very high air flowrates which may foster higher carbon efficiency and make gas heating value.

The cyclone model is capable of treating a very broad range of stoichiometries, including both coal combustion and fuel-rich gasification. The model results compare very favorably with the experimental results for the conditions studied thus far. Modeling of fuel-rich gasification would be improved by the inclusion of mechanisms for char oxidation by steam and carbon dioxide. The simple fluid mechanics treatment is adequate for the range of air flowrates considered herein; however, tests at significantly higher air flowrates may reveal weaknesses that will require a more detailed analysis.

A similar experimental/analytical investigation has been initiated for the jet reactor. An initial shakedown run has been completed and all apparent problems corrected. The emphasis in the next few months will be on obtaining data for combustion and fuel-rich gasification of coal in the jet reactor. Concurrently, the fluid mechanics model will be developed or adapted from existing computer programs.

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