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GASIFICATION IN PULVERIZED COAL FLAMES

Final Report (Part I). Pulverized Coal Combustion and Gasification in a Cyclone Reactor: Experiment and Model

By
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May 1979

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U. S. DEPARTMENT OF ENERGY

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Department of Energy
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Report No. PURDU-CL-79-04

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LIST OF SYMBOLS

A	frequency factor ($\text{g/cm}^2\text{-s-atm}$)
A_j	thermocouple junction surface area (m^2)
A_p	particle surface area (ft^2)
A_v	frequency factor (sec^{-1})
$(A/F)/(A/F)_S$	actual air to fuel ratio divided by the stoichiometric air to fuel ratio
a_c	char particle radius (ft, μm)
a_{coal}	coal particle radius (ft, μm)
a_c	critical particle radius (ft, μm)
B_v	activation energy ($^{\circ}\text{K}$)
B_1	frequency factor (sec^{-1})
B_2	frequency factor (sec^{-1})
C_v	char residual volatile mass fraction (lb/lbchar)
CFR	coal feed rate (lb/hr)
c_p	coal (or char) particle specific heat ($\text{BTU/lb-}^{\circ}\text{R}$)
$c_{p,j}$	specific heat of species j ($\text{BTU/lb-}^{\circ}\text{R}$)
$D(T,P)$	molecular diffusivity of oxygen (cm^2/s)
d	particle diameter (cm)
$\bar{d}$	characteristic particle diameter for Rosin-Rammler distribution (μm)
E	activation energy (kcal/gmole)
E_1	activation energy (kcal/gmole)
E_2	activation energy (kcal/gmole)

F_i	molar flowrate of species i (lbmole/hr)
f_i	coal mass fraction of species i
f_v	coal mass fraction volatilized
$f_{C,v}$	mass fraction of coal carbon volatilized
G_ϕ	axial flux of angular momentum
G_x	axial flux of linear momentum
H_p	total enthalpy of products (BTU/hr)
H_R	total enthalpy of reactants (BTU/hr)
H_2O_{in}	steam flow into the reactor (lb/hr)
HL	reactor percent heat loss
$\Delta H_{C,coal}$	coal enthalpy of combustion (BTU/lb)
$\Delta H_{f,coal}$	enthalpy of formation of coal (BTU/lb)
ΔH_{fi}	enthalpy of formation of species i (BTU/lb)
ΔH_{pr}	difference in sensible enthalpy between products and reactants (BTU/lbcoal)
$\Delta \bar{H}_{C,CHONS}$	enthalpy of combustion of ash-free coal (BTU/lbmole)
$\Delta \bar{H}_{C,i}$	enthalpy of combustion of species i (BTU/lbmole)
$\Delta \bar{H}_{f,CHONS}$	enthalpy of formation of ash-free coal (BTU/lbmole)
h	convection coefficient ($W/m^2 \cdot ^\circ K$), (BTU/hr-ft ² -°R)
$(h_T - h_{537})_i$	sensible enthalpy of species i with reference to 537°R (BTU/lb)
K_c	particle surface chemical reaction rate coefficient (cm/s)
K_D	oxygen diffusion rate (cm/s)
K_p	equilibrium constant based on partial pressures
k_g	gas thermal conductivity ($W/m \cdot ^\circ K$), (BTU/hr-ft-°R)
k_i	thermal conductivity of species i ($W/m \cdot ^\circ K$)
k_o	frequency factor (cm ³ /gmole-hr)

k_1	pyrolysis rate coefficient (sec^{-1})
k_2	pyrolysis rate coefficient (sec^{-1})
L	cyclone chamber length (ft)
L_t	cyclone exit throat length (ft)
l_t	throat tube length measured from the cooling coil (ft)
M	molecular weight
MBE	mass balance error (%)
$\dot{m}_g$	product gas mass flowrate (lb/hr)
$\dot{m}_i$	mass flowrate of species i (lb/hr)
$\dot{m}_{\text{char}}$	char flowrate (lb/hr)
$\dot{m}_{\text{coal}}$	coal feed rate (lb/hr)
N_j	number flowrate of particles of radius r_j
Nu_f	Nusselt number evaluated at the film temperature
P	pressure (atm)
P_f	particle force balance factor
PFR	plug flow reactor
PSR	perfectly stirred reactor
Q	make gas heating value (BTU/scf)
Q_C	heat of combustion of carbon (BTU/lb)
Q_{CO}	heat of combustion of CO (BTU/lbmole)
Q_v	ratio of maximum volatiles yield to ASTM proximate volatiles yield
Q_{coal}	lower heating value of coal (BTU/lb)
$Q_{p,c}$	convection heat transfer rate to particle (BTU/lb)
$Q_{p,r}$	radiation heat transfer rate to particle (BTU/lb)
$\dot{Q}_c$	convection heat transfer rate to T/C (watts)
$\dot{Q}_r$	radiation heat transfer rate to T/C (watts)

$\dot{Q}_{\text{chem}}$	chemical heat release due to coal combustion (BTU/hr)
$\dot{Q}_{\text{in}}$	total energy input to reactor (BTU/hr)
$\dot{Q}_{\text{loss}}$	reactor heat loss rate (BTU/hr)
$\dot{Q}_v$	heat released due to volatiles combustion (BTU/hr)
R_t	cyclone exit throat radius (ft)
R_1	cyclone chamber radius (ft)
R	universal gas constant
RR	weight percent of coal of size greater than d
r_c	rate of carbon oxidation (lbmole/hr-ft ³)
r_j	radius of particle j (ft, μm)
r_{CO}	rate of CO oxidation (lbmole/hr-ft ³)
S	swirl number
SD	steam decomposition (%)
s	char swelling factor
T	temperature ($^{\circ}\text{K}$, $^{\circ}\text{R}$)
T_c	cooling coil surface temperature ($^{\circ}\text{K}$)
T_f	flame temperature ($^{\circ}\text{R}$)
T_g	gas temperature ($^{\circ}\text{K}$)
T_o	pressure vessel temperature ($^{\circ}\text{R}$)
T_p	particle temperature ($^{\circ}\text{R}$)
T_r	initial reactant temperature ($^{\circ}\text{R}$)
T_t	throat tube temperature ($^{\circ}\text{K}$)
T_w	reaction chamber wall temperature ($^{\circ}\text{R}$)
T/C	thermocouple
t	time (sec)

V_{PFR}	PFR zone volume (ft ³)
V_{PSR}	PSR zone volume (ft ³)
$V_{PFR,1}$	distributed feed portion of PFR zone (ft ³)
$V_{PFR,2}$	portion of PFR zone enclosed by throat tube (ft ³)
ΔV_{PFR}	PFR zone volume increment (ft ³)
VM_o	ASTM proximate volatile matter (lb/lb dry a.f. coal)
$\dot{V}$	volumetric flowrate (ft ³ /s)
ΔW	coal particle fractional weight loss (lb/lb dry a.f. coal)
x	exponential fitting constant for a Rosin-Rammler distribution, PFR zone distributed feed parameter
X_i	mole fraction of species i
Y	make gas yield (lb make gas/lbcoal)
Y_p	combustible make gas yield (lb comb. gas/lbcoal)
y_i	mass fraction of species i
α_1	mass stoichiometric coefficient
α_2	mass stoichiometric coefficient
$\alpha_{1,m}$	modified mass stoichiometric coefficient
$\alpha_{2,m}$	modified mass stoichiometric coefficient
ϵ	chemical yield (lb gas/lb coal reacted)
ϵ_f	flame emissivity
ϵ_j	junction emissivity
ϵ_p	particle emissivity
ϵ_v	pressure vessel emissivity
ϵ_w	chamber wall emissivity
η_c	carbon efficiency (%)
η_{cg}	cold gas efficiency (%)

η_{hg}	hot gas efficiency (%)
Λ	gravimetric stoichiometric coefficient (g-C/g- O_2)
μ	gas viscosity ($lb_m/ft-s$), ($kg/m-s$)
ρ	coal density (lb_m/ft^3)
ρ_c	char density (lb_m/ft^3)
ρ_g	gas density ($lbmole/ft^3$)
σ	Stefan-Boltzmann constant ($w/m^2-^{\circ}K^4$), ($BTU/hr-ft^2-^{\circ}R^4$)
ω_c	char carbon mass fraction
ω_p	combustible mass fraction

ABSTRACT

A unified experimental and analytical study of pulverized coal combustion and low-BTU gasification in an atmospheric cyclone reactor was performed. Experimental results include several series of coal combustion tests and a coal gasification test carried out via fuel-rich combustion without steam addition. Reactor stability was excellent over a range of equivalence ratios from .67 to 2.4 and air flowrates from 60 to 220 lb/hr. Typical carbon efficiencies were 95% for air-rich and stoichiometric tests and 80% for gasification tests. 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%, respectively. The corresponding product gas heating value was 70 BTU/scf.

A macroscopic model of coal combustion in the cyclone has been developed. Fuel-rich gasification can also be modeled through a gas-phase equilibrium treatment. Fluid mechanics are modeled by a particle force balance and a series combination of a perfectly stirred reactor 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, gas composition and temperature and reactor heat loss; 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.

I. INTRODUCTION

Rapidly dwindling oil and natural gas supplies and their inevitable escalation in price necessitate a substantial increase in the use of America's vast coal reserves. Economic considerations and concern for the environment require that processes for enhanced coal utilization be both efficient and clean. Coal is looked upon as a potential source for liquid and gaseous fuels, chemical feedstocks and cheap conversion to electrical energy; thus a wide variety of coal conversion processes is called for.

Interest in gasification of coal has increased substantially in recent years. Three types of gas may be produced in a coal gasification process: synthetic natural gas (900-1050 BTU/scf), synthesis gas (250-400 BTU/scf), and power gas (100-250 BTU/scf). Techniques for producing all three varieties of gas are receiving much well-deserved attention. The future for power gas usage in combined cycle generating stations appears particularly bright (National Academy of Sciences, 1977).

Coal gasification techniques can be conveniently classified as fixed bed, fluidized bed and entrained flow processes. The advantages and disadvantages of each are summarized in Table 1. The work described herein is devoted toward the development of entrained flow coal gasification processes using developed coal burner technology to efficiently produce power or synthesis gas. Two reactor configurations are considered: the cyclone or vortex tube (Figure 1) and the confined jet (Figure 2). Both reactors use swirling flow and separate reactant feeds to promote a separation of reaction zones within a single chamber: exothermic coal combustion reactions occur in the outer annular regions, driving endothermic steam-carbon reactions that occur in the core of the chamber (Lenzer et al., 1976).

Table 1. Reactor Types for Coal Gasification (Laurendeau, 1975)

<u>Type</u>	<u>Advantages</u>	<u>Disadvantages</u>
Fixed	Developed technology, counter-current flow, high pressure operation	Non-uniform flow, clinker formation, temperature control, ash removal, tar formation, low capacity, coal fines unacceptable, high H ₂ O levels
Fluidized	Solids handling, uniform temperature, gas-solid contact, countercurrent flow, <u>in situ</u> sulfur removal, high gasification rate	Pretreatment of caking coals, multistaged beds, carbon efficiency, ash disposal
Entrained	Highest volumetric reaction rate, slagging conditions, gas-solid contact, coal type irrelevant, high product temperature, compatible with coal slurries and froth flotation	Ash separation, temperature control, co-current flow, coal pulverization

Figure 1. Cyclone Reactor Schematic (Thomas, 1978)

Figure 2. Concentric Jet Gasifier Schematic (Thomas, 1978)

This report is concerned primarily with the development, testing and modeling of the cyclone reactor as a coal combustor. Gasification via fuel-rich combustion, a convenient intermediate step and a promising technology in its own right (Traenckner, 1953), is also considered. The relevance of the current work, the efforts of other investigators in similar fields and basic concepts of reactor modeling are discussed in Chapter II. Chapter III includes a detailed description of the cyclone reactor and other important systems in the test facility. A description of the cyclone mathematical model and a summary of the important model results are presented in Chapter IV. The experimental results achieved to date are presented and compared with the model results in Chapter V. Conclusions and recommendations are presented in Chapter VI.

II. CYCLONE REACTOR APPLICATIONS AND MODELING

The cyclone reactor possesses several unique characteristics that make it attractive for coal conversion processes. Long particle residence times, slagging operation and intense particle-gas mixing are three features that are potentially useful in gasification systems. Cyclone combustors have been commercially available since 1944 (Steam, 1963); experimental studies with cyclone gasifiers date back to at least 1938 (Perry et al., 1950). The current rebirth of interest in coal gasification has spawned new cyclone experimental work (Lenzer et al., 1976; Joubert, 1978). Efforts are also underway toward modeling cyclone reactors (Mehta, 1976; Lewellen et al., 1977; Chung and Smith, 1978; Kane and McCallister, 1978; Thomas, 1978). The model of Thomas is of special interest since it was developed for the cyclone built for this project; it will be described in some detail along with proposed changes to make it more realistic.

A. Relevance of Coal Gasification and Cyclone Technology

1. The Need for Clean Fuels from Coal

There is widespread belief that the world's readily recoverable oil and natural gas reserves are being rapidly depleted and will become scarce by the year 2000. Long term solutions to the world's energy problems such as solar and fusion power cannot be expected to make significant contributions until well into the next century (Hirschfeld, 1978). Expanded coal usage in an environmentally acceptable manner is an absolute necessity if a dependable and affordable supply of energy is to be maintained.

The conversion of coal to gaseous fuels is a technology that is being vigorously pursued as a means of increasing coal usage. Attention has

focused on three categories of coal-derived gas: power gas, synthesis gas and synthetic natural gas. Their properties are summarized in Table 2. While potential applications for all three exist, the primary thrust of this investigation is toward the development of power gas.

Power gas is typically produced by reacting coal with air and steam. A portion of the coal is burned to provide heat to drive the endothermic steam-carbon and CO_2 -carbon reactions which yield hydrogen and carbon monoxide. The product gas is heavily diluted with nitrogen from the air. Power gas production enjoys an economic edge over other production schemes primarily because of its simplicity: no oxygen plant is required and shift conversion and methanation units are of course unnecessary.

The low energy content of power gas makes it impractical for pipeline distribution over appreciable distances; only those applications (industrial heating/steam-raising, power generation) where the gasifier can be located on site are potentially economical. The combined cycle power plant is a leading candidate for future use of low BTU gas (National Academy of Sciences, 1977). Oil and natural gas-fired combined cycle units have already proven themselves commercially; they are about one percent more efficient than the best boiler-steam turbine units (Mellor, 1978). This competitive edge should increase with the development of gas turbines capable of higher inlet gas temperatures. A low BTU gasifier-combined cycle plant uses about 50 percent less water than a conventional power plant (National Academy of Sciences, 1977). This is important in arid Western states where coal is abundant but water is scarce.

Low BTU gasifiers are also attractive from an environmental viewpoint. Fuel-bound sulfur and nitrogen are typically converted to H_2S and NH_3 , respectively, in the hydrogen-rich gasifier, in contrast to the SO_2 and NO_x that form during coal combustion. Commercially proven processes are available for the removal of H_2S and NH_3 from the product gas; however, they are limited to a gas temperature range of 50 to 120°C . Processes which operate over a range of 540 to 900°C are more efficient and are currently under development (National Academy of Sciences, 1977). The gas cleanup process is easier if the gasifier operates in a slagging

Table 2. Summary of Gasification Processes

<u>Process</u>	<u>Low BTU</u>	<u>Inter. BTU</u>	<u>High BTU</u>
Product	Power Gas	Synthesis Gas	Synthetic Natural Gas
Primary Constituents	N ₂ , CO, H ₂	H ₂ , CO	CH ₄
Energy Content ($\frac{\text{BTU}}{\text{scf}}$)	150	400	950
Cost (\$/10 ⁶ BTU)*	2.40 ^a	3.20 ^a	4.50 ^b
Conversion Efficiency (%)	90 ^c	80 ^c	65 ^c

*Based on 1978 dollars

^aAdapted from National Academy of Sciences (1977)

^bAdapted from Hammond and Baron (1976)

^cTillman (1976)

mode because most of the ash (roughly 85% for cyclones) is removed as molten slag.

2. Fundamental Cyclone Behavior

Cyclone fluid mechanics and the chemistry of coal gasification have been covered in detail elsewhere (Strickland, 1973; Lewellen et al., 1977; Schmidt, 1970; von Fredersdorff and Elliott, 1963); only a brief overview will be presented here. The parameter that most conveniently characterizes the fluid mechanical behavior of the cyclone is the swirl number S defined as the ratio of the axial flux of angular momentum (G_ϕ) to the flux of linear momentum (G_x), nondimensionalized by the chamber exit radius (r_e):

$$S = G_\phi / G_x r_e \quad (2-1)$$

In a parametric study of cyclone gasifiers Chung and Smith (1978) found the swirl number to be more significant than the char gasification kinetic parameters due to its influence on turbulence levels and mixing rates. Typical cyclone swirl numbers range from 10 to 20 and are much higher than those found for concentric jet burners (Syred and Beer, 1974).

Swirling flow and separate reactant feeds are used in the cyclone gasifier to promote a separation of reaction zones. Coal and air are fed into the cyclone tangent to the wall near the top of the chamber (Fig. 1). The stoichiometry is controlled so that a portion of the coal burns in the outer annular portion of the reactor. Steam is fed axially into the chamber and reacts endothermically with the coal particles in the core of the reactor. The exothermic coal combustion reactions serve the dual purpose of promoting slagging conditions while providing energy to drive the endothermic gasification reactions.

Many of the features that make the cyclone uniquely suited to coal gasification are elucidated by a discussion of particle behavior. Upon entering the cyclone the coal particles are thrown against the molten slag-covered walls by centrifugal forces (Semenov and Semenenko, 1969). The majority of slags are non-wetting and the particles return to the

fluid stream where they are accelerated by viscous forces only to be thrown once again into the wall. This particle-slag interaction continues until the particles are small enough to be entrained by the exiting gas flow. This interaction is beneficial in many respects. Particle-gas relative velocities are high, leading to rapid reaction rates. Molten slag which accumulates on the particle surface is effectively transferred to the walls. Carbon efficiencies are high because the particles remain near the walls for long periods under the influence of swirling flow. Particle residence times are also enhanced by numerous axial flow reversals as observed by Agrest in a quartz rotary flow furnace (Schmidt, 1970). By varying the amount of swirl, particle residence times in the combustion and gasification zones of the reactor can be varied; this is a measure of control that is not found in unswirled flows (Laurendeau, 1978a).

B. Commercial and Experimental Cyclone Reactors

The available literature on cyclone reactors is sparse and in some cases of dubious quality, reflecting the humble niche occupied by cyclones until very recently. Early tests showed that cyclones could burn and even gasify "difficult" fuels such as brown coals and vegetable wastes (Steam, 1963; Schmidt, 1970); however, concern about air pollution and the availability of inexpensive natural gas made the use of such fuels impractical in most circumstances. In view of the current energy situation, it is appropriate that the long-ignored virtues of cyclone reactors are once again the subject of technological study (Table 3).

Boilers with cyclone burners were introduced by the Babcock and Wilcox Company in 1944. The B & W cyclones retained 85 to 90 percent of the coal ash in the form of slag; thus fouling of heat transfer surfaces and stack particulate emissions were greatly reduced. Coals that were troublesome in other boilers (high ash content, low ash fusion temperature) were handled easily in cyclones (Steam, 1963). Unfortunately the high gas temperatures and intense combustion produced by cyclone burners lead to unacceptable NO_x emissions; therefore cyclone-fired boilers are not used on a wide scale in the United States today.

Table 3. Investigations of Cyclone Reactor Performance

<u>Reference</u>	<u>Fuel and Process</u>	<u>Coal Feed Rate (lb/hr)</u>	<u>Size and Geometry (dimension: inches)</u>	<u>Carbon Efficiency (%)</u>
Steam (1963)	Cr. coal combustion	40,000	D = 108; L = 144; horiz. axis; tangential feed	~ 100 (no data)
Schmidt (1970)	Plant residue combustion	10,000	D = 75; L = 100; horiz. axis; tangential feed	-----
Perry et al. (1950); Elliott et al. (1952)	Pulv. coal gasification (O ₂ /H ₂ O)	40-100	D = 24; L = 36; vertical axis; axial feed	65(nonslagging) 80(slagging)
Traenckner (1953)	Pulv. coal gasification (air; O ₂ /H ₂ O)	1250	D = 32; L = 40; vertical axis; tangential feed	80(no recycle) 95(recycle)
Yagi and Kunii (1957)	Pulv. coal gasification (O ₂ /H ₂ O)	2-5	D = 8; L = 13; vertical axis; tangential feed	85-98
Hoy et al. (1958)	Cr. coal combustion	1800	D = 36; L = 36; vertical axis; tangential feed	96
Kalishevskii and Ganchev (1966)	Pulv. coal combustion		D = 24; L = 27; horiz. axis; tangential feed	-----
Jackson (1967)	Pulv. coal combustion	1-10	D = 4; L = 18; vertical axis; tangential feed	-----
Joubert (1978)	Pulv. coal combustion, gasification (air)	100	D = 12; L = 16; vertical axis; tangential feed	95
Barnhart et al. (1978)	Pulv. coal combustion, gasification (air)	7-28	D = 6; L = 10; vertical axis; tangential feed	80-98

The capability of cyclones to handle difficult fuels is further illustrated by Schmidt (1970), who describes 18 Siemens-Agrest rotary flow furnaces burning such unlikely fuels as grape seeds, sunflower hulls and coffee bean wastes. Commercial interest in cyclone combustors has also been fostered by magnetohydrodynamic (MHD) research (Way, 1974). The ideal MHD burner would produce an exceedingly hot ($2600 - 2800^{\circ}\text{K}$), low particulate level gas stream with a low hydrogen content; a coal- or char-burning cyclone with sufficient air or oxygen preheat can be used to produce such a stream.

The first investigation of pulverized coal gasification in a cyclone reactor was carried out by the Fuel Research Board in England in 1938. Pulverized coal combustion in a cyclone was studied in 1946 at Battelle Memorial Institute for locomotive applications. The results of these two investigations prompted researchers at the U.S. Bureau of Mines to build and test a laboratory scale oxygen-blown gasifier (Perry et al., 1950; Elliott et al., 1952). Their early efforts still rank as one of the most significant and thorough studies of cyclone coal gasification.

Experiments were carried out in a vertical axis cyclone 24 inches in diameter (Fig. 3). Chamber height could be varied from 2 to 36 inches; best results were achieved with the maximum height. Tests were conducted at atmospheric pressure with coal feed rates up to 100 lb/hr. Steam/coal ratio was typically .55 lb/lb, and oxygen/coal was varied from .6 to 1.0 lb/lb. Steam and oxygen were preheated to 1300°F .

An objective of the first series of tests was the avoidance of slagging conditions. As a consequence of this precaution and poor coal feeder operation, carbon efficiencies were low, typically 50 to 75 percent (Perry et al., 1950). Later tests with a modified reactor operating under slagging conditions yielded carbon efficiencies over a range of 60 to 90 percent (Elliott et al., 1952). In both cases carbon efficiency increased almost linearly with oxygen/coal ratio.

An important analytical result of this study was a method of predicting adiabatic reactor performance based on the observed performance of laboratory reactors (Elliott et al., 1952). Perry et al. (1950) also developed a particle force balance analysis that has since been adapted by Thomas (1978) for use in a mathematical model describing the cyclone of this investigation (see Section II.C.3).

Figure 3. The Vortex Coal Gasifier of Perry et al. (1950) and Elliott et al. (1952)

Investigators in Germany meanwhile were developing the so-called Ruhrgas process (Traenckner, 1953). The reactor was a vertical axis slagging cyclone operated at atmospheric pressure. Dust in the product gas was trapped and recycled to improve carbon efficiency, typically increasing its value from 80 to 95 percent. The limited experimental results are very promising: a low-BTU gas made via fuel-rich gasification with preheated air (1700°C) had a heating value of 100 BTU/scf; the corresponding cold gas efficiency was 61%. A medium-BTU gas (268 BTU/scf) was produced with a cold gas efficiency of 75% via an oxygen/steam blown process (National Academy of Sciences, 1977). A 100 ton per day commercial plant was eventually built but operated for only a few years.

Yagi and Kunii (1957) demonstrated the feasibility of conducting coal gasification experiments in a laboratory-scale reactor (Table 3). Tests were conducted in a vertical axis cyclone at atmospheric pressure with tangential reactant feed. Coal was gasified with steam and oxygen and a small amount of primary air, yielding carbon efficiencies of 85 to 98 percent. A throat tube which projected into the reaction chamber kept unreacted particles from leaving. Ash retention was 70 to 80 percent; the molten slag was simply allowed to accumulate in the bottom of the reactor during a run, apparently with no detrimental effects.

Laboratory scale cyclone combustion tests have also been conducted by Hoy et al. (1958), Kalishevskii and Ganchev (1966), Jackson (1967) and Joubert (1978). High ash retention through slagging conditions and high carbon efficiency were goals common to all these efforts. In fuel-rich combustion tests ($\phi = 1.3$) Joubert achieved ash retentions and carbon efficiencies above 95% with a Rosebud seam coal. A secondary air preheat temperature of 2800°F was an important factor. Summaries of the aforementioned programs and the current investigation are presented in Table 3.

In spite of the limited amount of information available, it is clear that cyclone reactors show great potential for coal combustion and gasification processes. It is also clear that much more work, both experimental and analytical, must be done before a fundamental understanding of cyclone behavior is achieved. Experiments should be directed

toward gasification at high pressure, internal species and temperature mapping and trials of long duration to demonstrate high reliability. A common defect of the studies cited is the apparent absence of any substantive data analysis or reactor modeling; in some cases such fundamental parameters as carbon efficiency are not even reported. A unified experimental and analytical approach is the optimum tool for moving cyclone reactors closer to commercial application.

C. Cyclone Reactor Modeling

Mathematical models of cyclone reactors have been developed in recent years in an effort to more fully understand the complexities of the coal conversion process. The more general topic of pulverized coal combustor modeling is covered by Thomas (1978). This review will focus on cyclones in particular, beginning with a brief description of reactor mixing theories.

1. Reactor Mixing Theories

Pratt (1974) divided mixing theories into two basic categories, the mechanistic theories and the population balance theories. Mechanistic theories model turbulent flow phenomena via the governing differential equations. A finite difference approach is used to solve the system of equations. In theory, turbulence effects can be modeled directly by choosing a mesh size much smaller than the smallest eddy of interest and describing in detail the entire flow field; more often, an empirical turbulence model is chosen to approximate the gross fluid behavior. In either case the mechanistic approach quickly becomes intractable when considering a three dimensional, two phase, chemically reacting system.

The population balance theories, by virtue of their simplicity, offer a more promising means of investigating cyclone behavior. Two theoretical models of special interest are the perfectly stirred reactor (PSR) and the plug flow reactor (PFR). In perfectly stirred reactor theory, the incoming reactants enter a volume in which mixing occurs at an infinite rate. All properties of the reactor volume are uniform and

equal to those of the exit stream. The PSR model is applicable when the reactants are spread throughout the reactor volume in much less time than the mean residence time. Clearly internal heat transfer is not considered in PSR theory; however external heat transfer can be included (Thomas, 1978).

Plug flow reactor theory assumes infinite mixing in the radial direction and no mixing in the axial direction (the direction of flow). Thus any cross section normal to the flow has uniform properties and velocity. The absence of mixing in the axial direction is often unrealistic in combustion systems; thus it becomes necessary to modify the PFR framework by including backmixing and axial heat transfer effects (Thomas, 1978).

Combinations of perfectly stirred reactors and plug flow reactors are often used to model a single combustion system. In this fashion the relatively simple population balance theories can be used to model extremely complicated reactor configurations.

2. Current Cyclone Reactor Models

Five models for the combustion of pulverized coal in a cyclone reactor have been found in the literature. The models have surprisingly little in common; they reflect the wide variety of approaches that are available in the modeling process. Four of the models will be discussed briefly. The fifth, that developed by Thomas (1978), will be reviewed in more detail since it forms the core of the model to be presented in this report.

Mehta (1976) modeled a pulverized coal cyclone combustor as part of a multi-stage coal gasification process. The combustor was modeled as a perfectly stirred reactor operating at a design temperature of 3200⁰F. The exhaust gas composition and temperature are determined by an equilibrium calculation. External heat transfer in the form of radiation to the walls, slag hole and exhaust throat is also modeled. No pyrolysis or kinetics effects are included. Particle burnup is assumed to be complete except for a small portion of the carbon which is lost in the molten slag. No comparison with experimental results is reported.

Lewellen et al. (1977) developed a cyclone coal combustion model based largely on fluid mechanics and particle-gas interactions. Important output parameters from the model include carbon efficiency, ash retention, pressure drop and radiative and convective heat loss. This model can best be described as occupying the middle ground between the mechanistic and population balance theories. Pyrolysis and char particle combustion are only modeled in a crude fashion. A sophisticated fluid mechanics treatment, however, includes a four region model of the reaction chamber in which the basic conservation equations are simplified for each region by applying appropriate assumptions. The wall-adjacent region was found to be by far the most important since particle loading and chemical reactions are concentrated in this zone. Lewellen et al. report good agreement with limited experimental data from a cyclone operated by the Pittsburgh Energy Research Center.

Kane and McCallister (1978) modeled a cyclone char combustor through direct analysis of the governing mass, momentum and energy equations. The equations were nondimensionalized and an order of magnitude analysis was performed to determine the significant dimensionless parameters with an eye toward simplifying scale-up of laboratory cyclone reactors. Among the dimensionless groups found to be important are the swirl number, particle loading ratio, the Biot modulus and a reaction time-residence time ratio. This study suggests a useful correlation procedure, but the absence of any gasification chemistry or predictive potential is a defect.

Chung and Smith (1978) carried out a parametric analysis of a cyclone gasifier by developing broad assumptions giving closed form solutions to the continuity, momentum and species conservation equations. The energy equation was eliminated in favor of an estimated reactor temperature of 4000°R . Particles were assumed to reside only in the wall-adjacent region, making a detailed description of the bulk fluid flow unnecessary. Parameters that were systematically varied include the gasification rate coefficients, swirl number and coal mass fraction pyrolyzed. Swirl number proved to be of great importance through its effect on mass transfer rates since the gasification reactions were presumed to be diffusion controlled. A commonly cited virtue of swirl

burners is long particle residence time; however, the authors point out that increased residence time is beneficial only if the mass transfer rate is sufficient to keep gasification products swept away from the particle surface.

3. The Thomas Cyclone Model

Thomas (1978) developed a model for coal combustion in the cyclone reactor described in this report. The model consists of an instantaneous pyrolysis process followed by a perfectly stirred reactor and a plug flow reactor. Both heterogeneous char kinetics and carbon monoxide kinetics are included. The heat transfer model includes radiation and convection to the chamber walls, conduction through the insulating layers, and radiation and free convection from the vessel. The model predicts carbon efficiency, exhaust gas composition and temperature and percent heat loss. This section includes a description of the Thomas model, a brief summary of the results and suggested means of improving and extending the model.

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. Note that although the pyrolysis process is assumed to be instantaneous, a finite portion of the reactor volume is assigned to it. The major governing assumptions for each reactor zone are listed in Table 4. 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 temperature is calculated by assuming that the pyrolysis and PFR zones are adiabatic and that all heat losses come from the PSR zone.

The pulverized coal particles entering the pyrolysis zone are assumed to be moisture-free and follow a Rosin-Rammler size distribution. Intense radiation and convection heat the particles, driving off the volatile content and causing them to swell slightly (10%). The weight loss due to pyrolysis (40%) is assumed to be slightly greater than the proximate volatile matter, as determined by the standard ASTM

Figure 4. Cyclone Combustor Model Schematic (Thomas, 1978)

Figure 5. Hypothesized Cyclone Reaction Zones
(Thomas, 1978)

Table 4. Major Modeling Assumptions (Thomas, 1978)

Pyrolysis Zone

1. Input coal particles contain no moisture and follow a Rosin-Rammler size distribution.
2. Devolatilization is instantaneous with 40% of the coal mass released (dry basis).
3. All of the coal H, N, O and S is lost in pyrolysis; all ash is retained in the char.
4. Volatiles burn instantaneously to form H_2O , NO, SO_2 and CO; no CO_2 is formed.
5. Particles swell in diameter by 10%.
6. The pyrolysis zone is adiabatic for the nonisothermal case and isothermal for the constant temperature case.

PSR Zone

1. Particles entering the PSR zone, whose size is greater than a critical size, burn forming CO as the only product (CO_2 is only formed in the gas-phase reaction) until reaching the critical size. 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. The char ash is lost at a rate proportional to carbon combustion, such that the char composition remains constant throughout the reactor.
3. Homogeneous conversion of CO to CO_2 (and corresponding O_2 depletion) is calculated assuming the zone to be a micromixed perfectly stirred reactor.
4. All heat losses from the reactor occur in the PSR zone.
5. Gas dissociation is ignored.

Table 4. . (cont.)

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. Gas dissociation is ignored.

analysis. All the coal hydrogen, nitrogen, oxygen and sulfur volatilize; carbon makes up the rest of the volatile matter. The heating value of the volatiles is assumed equal to that of the char (fixed carbon and ash). The volatiles burn instantaneously to form H_2O , NO , SO_2 and CO . For the nonisothermal analysis, the pyrolysis zone outlet temperature is calculated from an energy balance. Molecular dissociation is not considered.

Following pyrolysis and volatiles combustion the reactants enter the perfectly stirred reactor zone. 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. Char and CO oxidation plus external heat transfer are the main features of the PSR analysis.

The extent of char oxidation 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):

$$a = \frac{3}{2} P_f (L - L_t) (R_1 - R_t) \frac{R_t}{R_1} (\mu / \pi \rho \dot{V} L)^{1/2} \quad (2-2)$$

where P_f is a particle force balance factor, L the chamber length, L_t the throat tube length, R_1 the chamber radius, μ the gas viscosity, ρ the particle density and $\dot{V}$ the volumetric flowrate. Char oxidizes in the PSR 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 factor is a fitting parameter which is adjusted to create agreement between the calculated 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 the critical radius a are assumed to be completely converted to CO in the PSR.

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

$$-\frac{d}{dt} [\text{CO}] = k_0 [\text{CO}] [\text{O}_2]^{1/2} [\text{H}_2\text{O}]^{1/2} \exp(-E/RT) \quad (2-3)$$

where k_0 is the pre-exponential factor, $[\text{CO}]$, $[\text{O}_2]$ and $[\text{H}_2\text{O}]$ are gas concentrations (g-moles/cm^3), E is the activation energy, R the universal gas constant, and T the temperature. Howard et al. (1973) recommend k_0 and E values of $1.3 \times 10^{14} \text{ cm}^3/\text{g-mole-s}$ and 30 kcal/g-mole , respectively. No previous pulverized coal combustion model has considered the homogeneous kinetics of CO combustion; they are treated here because of the short gas residence times.

A plug flow reactor was chosen for the exit region because of the lower levels of turbulence and the resemblance to pipe flow. Gases and a monosize particle distribution (a consequence of the PSR force balance analysis) enter the PFR in an evenly distributed manner over that portion of its length not enclosed by the throat tube. Carbon monoxide burnup is treated as in the PSR zone. Char oxidation to CO is assumed to occur under combined chemical and diffusion control, expressed as (Laurendeau, 1978b):

$$R_e = [\text{O}_2]/(1/K_D + 1/K_C) \quad (2-4)$$

where R_e is the reaction rate based on external surface area ($\text{g/cm}^2\text{-s}$), $[\text{O}_2]$ the bulk concentration of oxygen (g/cm^3), K_D the rate of oxygen diffusion to the particle surface (cm/s), and K_C the chemical reaction rate coefficient at the surface (cm/s).

For particles under $100 \mu\text{m}$, K_D can be calculated assuming a stagnant gas film around a spherical char particle (Laurendeau, 1978b). With temperature T and pressure P ,

$$K_D = 2 \Lambda D(T,P)/d \quad (2-5)$$

where Λ is the gravimetric stoichiometric coefficient (g-C/g-O_2), $D(T,P)$ the molecular diffusivity for oxygen (cm^2/s), and d the particle diameter (cm).

K_C is expressed by the Arrhenius expression

$$K_C = A \exp(-E/RT) \quad (2-6)$$

where A is the pre-exponential factor, and E , R , and T are as previously defined. For pulverized bituminous char, Smith (1971) found E and A to be 16 kcal/g-mole and $8 \text{ g/cm}^2\text{-s-atm}$, respectively for $1200 < T < 2270^\circ\text{K}$.

Chemical reactions in the PFR continue until the gases reach the cooled portion of the reactor exhaust at which point the products are assumed to be quenched. The effect of molecular dissociation is not considered.

The most important result of the model is the predicted behavior of carbon efficiency as a function of temperature, air flowrate and stoichiometry (Fig. 6). Carbon efficiency increases monotonically and at a nearly constant slope with temperature. In the PSR zone high temperature increases carbon efficiency by increasing the volumetric flowrate for a given mass flowrate, causing a decrease in the critical particle radius (Eqn. 2-2). Conflicting effects occur in the PFR zone: (1) char combustion speeds up because both the chemical and diffusion rates increase with temperature (Eqns. 2-2, 5 and 6) and (2) PFR zone residence time decreases due to increased volumetric flowrate. The PSR zone is responsible for the increase in carbon efficiency for fuel-rich conditions while the PFR zone dominates for fuel-lean conditions.

The effect of stoichiometry is negligible at low temperatures but becomes dominant as temperature increases. Stoichiometry comes into play only in the PFR zone through the linear dependence of char oxidation rate on oxygen concentration (Eqn. 2-4). At low temperature ($< 2400^\circ\text{R}$) the reaction rate is low, a negligible amount of carbon burns in the PFR, and the effect of stoichiometry is minimal. At high temperature, however, the reaction rate is much higher so a substantial amount of carbon burns in the PFR, especially when the oxygen concentration is high.

Increased flowrate produces opposing effects: (1) more char is burned in the PSR due to enhanced centrifugal effects and (2) less char is burned in the PFR due to decreased residence time.

Figure 6. Carbon Efficiency as a Function of Exit Temperature, Air Flowrate and Stoichiometry (Thomas, 1978)

The combined effect of all the trends illustrated in Fig. 6 is a spread in carbon efficiency of only about 6 percent, so to match the observed trends with experimental data would require very precise measurements. The range of values predicted is in very close agreement with both data taken at the Pittsburgh Energy Research Center (Joubert, 1978 - 93 to 97 percent) and in the present investigation (Chapter V).

For the nonisothermal case, exit temperature was found to peak predictably near stoichiometric (Fig. 7). Increased flowrate also enhanced the exit temperature since percent heat losses decreased. Predicted exit temperatures are significantly higher than those achieved experimentally due to the neglect of dissociation and the rather small predicted heat loss levels (typically 10 to 15 percent). Carbon efficiency peaks slightly on the air-rich side of stoichiometric since an overabundance of air reduces the exit temperature. Carbon efficiency increases with flowrate for the reasons given earlier.

The effect on carbon efficiency of changes in some of the model parameters is also shown in Fig. 7 for the case of 200 lb/hr air flowrate. Reducing the force balance factor P_f to 1.0 yields an increase of roughly 3 percent in carbon efficiency. Doubling the average input particle diameter has an almost identical effect, again due to the force balance treatment. Increasing the mass fraction volatilized also increases carbon efficiency due to the lower carbon mass fraction of the escaping particles.

It is appropriate now to list four shortcomings present in this model: (1) the incoming coal particles are assumed to be moisture-free; (2) pyrolysis kinetics are bypassed in favor of a constant weight loss model; (3) no check is made on the kinetic results to see if they overshoot the limitations imposed by equilibrium and (4) gasification via fuel-rich combustion cannot be modeled due to stoichiometric limitations. Since the rate of pyrolysis increases strongly with temperature, the effect of assuming a constant volatiles mass fraction is to overestimate the volatile yield at low temperature and to underestimate it at high temperature. The potential effect on carbon efficiency is obvious from Fig. 7. The high exit temperatures predicted by the model might be due in part to second law violations resulting from the kinetic treatment.

Air Flowrate

A - 100 lb/hr

B - 200 lb/hr

C - 300 lb/hr

Figure 7. Gas Exit Temperature and Carbon Efficiency Versus Input Stoichiometry (Thomas; 1978)

In the revised model to be presented in Chapter IV these factors will be dealt with in a simple fashion by (1) making minor changes to account for the coal moisture mass fraction; (2) developing a pyrolysis model which predicts weight loss as a function of reactor temperature; (3) checking the model kinetic results against a simple equilibrium model and (4) extending the range of stoichiometries that can be investigated to include gasification via fuel-rich combustion.

D. Rapid Pyrolysis of Pulverized Coal

1. Background and Relevance

The term volatiles applies to gaseous and tarry species that are evolved as a result of thermal decomposition of coal. The process of thermal decomposition is often called pyrolysis or devolatilization; these terms will be used interchangeably in this report. Renewed interest in coal conversion technologies has shed new light on the complex process of pyrolysis. Often, the objective is to optimize the quantity and makeup of the volatile matter evolved during a particular process (Anthony and Howard, 1976). This section will focus on the nature of the volatile matter, factors affecting its evolution and its importance in coal conversion processes.

It is erroneous to think of coal as being composed of well-defined amounts of volatile matter and fixed carbon (Badzioch and Hawksley, 1970). The yield of volatile matter during pyrolysis is primarily dependent upon particle size, heating rate, final temperature, total pressure and local gas-phase composition. The estimates of volatile matter and fixed carbon based on the standard proximate analysis of coal have no absolute significance, but nevertheless provide a useful relative measure (Field et al., 1967). The primary constituents of volatile matter are H_2O , H_2 , CO_2 , CO , hydrocarbon gases and tars. Solomon (1977) observed that the composition and structure of the tars are very similar to those of the parent coal, leading him to conclude that the tar molecules were "monomers" of the coal "polymer."

The quantity and composition of the volatile matter are determined by (1) the characteristics of the parent coal and (2) the conditions under which pyrolysis occurs. Solomon (1977) correlated the potential yield of the various volatile constituents with appropriate functional groups within the coal. Thus not only the ultimate analysis of the coal, but also its organic structure is significant. For a given coal, temperature is the factor which has the greatest effect on pyrolysis. Coals begin to devolatilize at about 400°C, and the extent of devolatilization increases with temperature up to about 1900°C (Smoot and Horton, 1977; Kobayashi et al., 1977; Kimber and Gray, 1967). The effect of heating rate is not yet determined. Badzioch and Hawksley (1970) report that yield and carbon content of the volatiles both increase with heating rate. Other investigators, however, report little or no effect (Anthony et al., 1976).

Particle size and total pressure affect volatiles yield because of the reactive nature of some of the volatile components. Volatiles yield is reduced when these intermediate components contact the particle matrix and react to form char or soot; thus low pressure and small, well dispersed particles, which tend to reduce the residence time of the intermediates within the particle, serve to increase the yield of volatile matter. Badzioch and Hawksley (1970) found that for particles less than about 100 microns the effect of particle size was negligible.

Pyrolysis is important both in direct coal combustion and in those processes which seek to produce a clean gaseous or liquid fuel from coal. Smoot and Horton (1977) emphasize the importance of coal volatiles in igniting and stabilizing pulverized coal-air flames. Anthony and Howard (1976) state that hydrogen reacts with devolatilizing coal several orders of magnitude faster than with the residual char, giving direct hydrogasification an edge over the other high BTU gas production cycles. In fixed and fluidized bed gasifiers, the volatiles are released in the top of the bed and become a part of the product gas, enhancing the gas heating value. The Garrett flash pyrolysis process and Combustion Engineering's low BTU process are two stage entrained gasifiers, both of which release the volatiles at a point where they become product gas constituents (National Academy of Sciences, 1977).

2. Experimental Investigations

Recent trends in pyrolysis experiments are toward more sophisticated diagnostic tools and improved apparatus that achieve faster heating rates and higher final temperatures. Two types of apparatus that have been used extensively are illustrated in Figs. 8 and 9. The first was developed by Badzioch and Hawksley (1970) and heats the particles by injecting them into a flowing, hot, nonreactive gas. In the second type of device the particles are held in a stainless steel mesh and heated electrically (Anthony et al., 1976).

Badzioch and Hawksley (1970) heated particles to 1000°C at rates of $25,000$ to $50,000^{\circ}\text{C}/\text{sec}$ for times ranging from 30 to 110 msec. They took data for eleven different coals and three size ranges. The observed weight loss was 1.3 to 1.8 times as great as the change in volatile matter found from the difference between the proximate volatile matter of the coal and that of the char. Kimber and Gray (1967) extended their results in the same apparatus to higher heating rates (10^5 - 10^6 $^{\circ}\text{C}/\text{sec}$) and final temperatures (1900°C) and found a second stage in the pyrolysis process during which the volatiles content of the char approached zero. No attempt was made to determine the makeup of the volatile matter.

Ubhayakar et al. (1977) pyrolyzed a Pittsburgh seam bituminous coal in a similar device in which the atmosphere was composed of hot combustion gases. The volatiles and char reacted with the hot gases, and the product gas composition was determined by infrared analyzers and gas chromatography. Volatiles yield was also measured by analysis and weight loss of the residual char. Discrepancies between the two methods led the investigators to propose the occurrence of soot-forming reactions in the gas phase.

Kobayashi et al. (1977) used the laminar flow furnace to pyrolyze a Montana lignite and a Pittsburgh seam bituminous coal at heating rates up to 2×10^5 $^{\circ}\text{C}/\text{sec}$ and final temperatures to 1800°C . Weight loss of both coals increased rapidly with temperature to a maximum of 63 percent of the original dry, ash-free coal (Fig. 10). Volatiles yield was measured directly by weighing particles before and after pyrolysis and by using ash as a tracer; results of the two methods were in good

Figure 2. Laminar Flow Furnace of Badzioch and Hawksley (1970)

Figure 9. Electrical Coal Heating Apparatus of Anthony et al. (1976)

Figure 10. Comparison of Calculated and Experimental Pyrolysis Weight losses (Kobayashi et al., 1977)

agreement, particularly for the bituminous coal. Particle residence time in the furnace was varied by changing the distance between the end of the feed tube and the top of the collector (Fig. 8). Although all the curves of Fig. 10 appear to approach asymptotic values, significant amounts of volatile matter remained in the char at all temperatures except 2100°K. The solid curves in Fig. 10 represent theoretical results to be discussed in the next section.

Working at MIT, Anthony et al. (1976) and Suuberg et al. (1978) used an electrical grid apparatus to pyrolyze a Pittsburgh bituminous coal and a Montana lignite, respectively. Heating rate, peak temperature, total pressure and residence time at peak temperature were all independently varied. Anthony et al. (1976) also investigated hydrogasification by conducting similar tests with various hydrogen partial pressures. No attempt was made to analyze the product gas. Suuberg et al. (1978) pyrolyzed in vacuum and in helium at one atmosphere and performed extensive analyses of the product gas.

Solomon (1977) conducted an extensive series of tests in vacuum with an electrical grid apparatus. Thirteen coals were studied over a temperature range of 300 to 1250°C. The quantity and composition of the gaseous products were determined for each run. Detailed analyses of the parent coal and tar were also conducted. Although the amount of a particular species evolved varied considerably from coal to coal, the temperature dependence for a given species was remarkably similar for all the coals tested. The amounts evolved were found to correlate well with certain organic structures in the parent coal.

Pyrolysis has also been studied in a peripheral sense by several investigators in other areas of coal research (Smoot and Horton, 1977; Smith and Smoot, 1978; Howard and Essenhig, 1966). Their studies provide valuable insight into the integration of the pyrolysis process with the overall mechanism of coal conversion.

3. Analytical Models

Virtually all the pyrolysis models mentioned heretofore were coordinated experimental/analytical efforts. In each case the nature of the

proposed model was strongly influenced by the conditions tested and the data available for a given condition. The four most significant analytical models are summarized in Table 5 and are described in some detail in this section.

Badzioch and Hawksley (1970) correlated their experimental data for weight loss with a single equation containing four fitting parameters, all of which are functions of coal carbon content. Their expression for weight loss ΔW as a fraction of dry ash-free coal is

$$\Delta W = Q_V VM_0 (1 - C_V) (1 - \exp\{-A_V (\exp(-B_V/T))t\}) \quad (2-7)$$

where Q_V is the ratio of maximum yield to ASTM proximate volatiles yield, VM_0 the ASTM proximate volatile matter (dry ash-free), C_V the char residual volatile mass fraction, A_V the frequency factor (sec^{-1}), B_V the activation energy ($^{\circ}\text{K}$), T_V the temperature ($^{\circ}\text{K}$) and t the decomposition time (sec). Values of Q_V range from 1.3 to 1.8 and increase linearly with coal carbon content. For weakly swelling coals a constant value of $C_V = .14$ is adequate; for highly swelling coals C_V is a function of temperature. Typical values of A_V and B_V are $3 \times 10^5 \text{ sec}^{-1}$ and 8900°K , respectively. In spite of the fact that extrapolation of Eqn. (2-7) above 1000°C is not recommended, the work of these investigators appears often in the literature and their correlation is widely used.

The model of Kobayashi et al. (1977) is an effective compromise between the very simple model of Badzioch and Hawksley (1970) and the complex model of Anthony et al. (1976). The model consists of two competing overall reactions:

$$k_1 = B_1 \exp(-E_1/RT) \quad (2-9)$$

$$k_2 = B_2 \exp(-E_2/RT) \quad (2-10)$$

Table 5. Pulverized Coal Rapid Pyrolysis Models

<u>Reference</u>	<u>Coals Investigated</u>	<u>Temperature Range (°C) and Heating Rate (°C/sec)</u>	<u>Model Description and Parameters</u>
Badzioch & Hawksley (1970)	10 Bituminous Coals, 1 Semianthracite	400-1000 25,000-50,000	Single equation overall weight loss model. Parameters include frequency factor, activation energy, char residual volatile content, and ratio of maximum volatiles yield to ASTM proximate volatiles content.
Kobayashi et al. (1977)	Montana Lignite Pittsburgh Seam Bituminous	700-1800 10^4 - 2×10^5	Overall weight loss model consisting of two parallel competing reactions representing low and high temperature yields. Parameters include frequency factors, activation energies, and mass stoichiometric coefficients for each reaction.
Anthony et al. (1976)	Pittsburgh Seam Bituminous	400-1100 65-10,000	Overall weight loss model employing a distribution of activation energies. Parameters include mean activation energy and standard deviation, frequency factor, and various quantities dealing with char deposition rate and pressure dependence.
Solomon (1977)	12 Bituminous Coals, 1 Lignite	300-1250 600	Yields of 7 different species are modeled independently. Tar yield competes with the evolution of gaseous volatile species. Parameters include frequency factor, activation energy, and yield at infinite time for each species.

where α_1 and α_2 are mass stoichiometric coefficients, B_1 and B_2 frequency factors and E_1 and E_2 activation energies. Low temperature yield is determined entirely by reaction (1) since activation energy E_2 (40 kcal/gmole) prevents significant yield via reaction (2). At high temperature reaction (2) takes over, providing excellent agreement with experimental values (Fig. 10). Weight losses from the lignite and bituminous coals were matched equally well with a single set of parameters.

Anthony et al. (1976) propose a model that includes a statistical distribution of activation energies for the pyrolysis of coal. A wide range of activation energies is an appropriate tool for modeling coal pyrolysis, which includes a multitude of independent and competing reactions. By choosing a Gaussian distribution only two parameters need be specified to describe the entire range of activation energies. The authors differentiate between reactive and nonreactive volatiles and include pressure and molecular diffusion effects, arriving at a truly formidable expression for volatiles yield which includes eight system parameters. Agreement between experiment and theory is excellent; however, extrapolation to different coals and reactor configurations would be difficult.

Solomon (1977) developed a model in which the time and temperature dependent evolution of each of the volatile species is calculated independently. The model is based on the observation that although the amount of a given species evolved varies from coal to coal the species profile as a function of temperature is strikingly similar for all coals. Thus a single set of kinetic parameters for each species can be used for all coals. The amount of a given species that will pyrolyze from a given coal is determined by the organic structure of the parent coal. Tar and gas production are modeled as competing processes. Since Solomon's work was done in vacuum no pressure effects are included.

4. Features of the Proposed Model

The pyrolysis model to be developed must meet the dual constraints of being realistic and accurate while being compatible with the rest of the cyclone mathematical model. The rate of evolution of volatile species

will thus be modeled after Kobayashi et al. (1977). The Kobayashi model is applicable to the full range of temperatures encountered in the cyclone and is readily implemented. No residual volatile matter will remain in the char; in particular, all coal hydrogen, nitrogen, oxygen and sulfur will pyrolyze. Particle heating rate will be calculated via a simple radiation-convection heat transfer model. Full details of the pyrolysis model are presented in Chapter IV.

III. FACILITY DESIGN AND CONSTRUCTION

A. Test Facility

The coal gasification facility is located at the Combustion Laboratory, Thermal Sciences and Propulsion Center, Purdue University. The heart of the facility is an explosion-proof test cell which houses the cyclone and jet reactors, coal feeder and flow network (Fig. 11). Adjacent to the test cell is a control room from which the reactors are operated and in which the mass spectrometer and flow and temperature monitoring stations are located. A large observation window is located between the two rooms. The reactant feed and exhaust networks and the data acquisition systems serve either reactor interchangeably to eliminate redundancy. Support buildings not shown on Fig. 11 include a block structure immediately behind the test cell which houses an electric boiler and a nearby cell used for coal preparation and storage.

B. Cyclone Reactor

1. Design Considerations

Table 6 lists the important factors that were considered in the design 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. The cyclone chamber radius of 3 inches was chosen to match industrial coal throughput rates and to allow probe insertion with minimal flow disturbance. A more thorough discussion of the cyclone design can be found in Lenzer (1977) and George et al. (1977).

Figure 11. Gasification Facility Schematic (George, 1978)

Table 6. Cyclone Design and Performance Characteristics

Vertical Axis

Slagging Reactor

Number of Tangential Nozzles:	4
Chamber Radius:	3 in.
Length to Diameter Ratio:	1.67
Swirl Number:	17.5
Design Pressure:	20 atm
Maximum Coal Throughput:	180 lb/hr-ft ³
Heat Release at Maximum Throughput*:	1.8×10^6 BTU/hr ft ³

*coal heating value - 10,000 BTU/lb

2. Construction Details

Figure 12 is an assembly drawing showing the current configuration of the cyclone. The walls of the reaction chamber are made of Babcock and Wilcox Kaocrete castable refractory. The sections are held together with Satanite, a slag-resistant high alumina cement (A.P. Green Refractories Co.). The slag port in the bottom section of refractory expands to improve slag flow. A methane torch fires into the reaction chamber through the top to preheat the chamber and to ignite the incoming coal/air mixture. Air and coal enter the chamber through four equally spaced sets of tangential concentric stainless steel tubes. Gases pass out of the reactor through a throat tube which projects into the reaction chamber to prevent unreacted particles from leaving the chamber. The exhaust line consists of a carbon steel reducing tee which is cooled by an internal cooling coil and a water jacket. Exhaust gases flow through the branch of the tee into water-jacketed exhaust piping (not shown). The top of the exhaust tee is capped, with provisions for a sight glass and sampling probe insertion.

The refractory sections are surrounded by four quarter-cylindrical heating elements (Electro-Applications, Inc.) for chamber preheat. Feedback thermocouples attached to the heaters and monitoring thermocouples imbedded in the refractory can all be removed and replaced during a test if necessary. The annulus is heavily insulated with Kaowool bulk insulation (Babcock and Wilcox, Inc.) and is maintained at a pressure slightly higher than that of the reaction chamber. The pressure vessel consists of a 24 inch steel pipe with a three inch plate on the bottom and a flange on top. A more complete description of the cyclone vessel may be found in Lenzer (1977) and George et al. (1977).

C. Control and Monitoring Systems

1. Flow and Temperature Monitoring

The flowrate and temperature of all reactants plus the exhaust gas are monitored periodically during testing. Various sampling system temperatures are closely watched to prevent water vapor condensation;

reactor shell and refractory temperatures are monitored for safety reasons. All system temperatures are measured with type K chromel-alumel thermocouples connected to a direct temperature readout via a 40 position thermocouple switch (Omega Engineering models KC175 and OSW5-40, respectively).

Methane and ignition air flowrates are monitored with rotameters (Brooks Instruments, Inc.). The gas pressures at the rotameters are measured with Dwyer Magnehelic gages. Primary and secondary air flowrates are measured with conventional orifice flow meters. The orifice plates and retaining blocks are made of stainless steel to ASME specifications and are calibrated against ASME standard orifices. Manometers and Bourdon tube pressure gages are used to monitor differential and gage pressures, respectively. Details of the orifice meter design and calibration are presented in George et al. (1977).

2. Coal Feeding and Conveying System

Fabrication and calibration of the coal feeding network was a considerable undertaking. Preliminary tests under entrained conditions yielded erratic results, which occasionally led to unsafe conditions. Through further testing, however, a reliable procedure for feeding coal was established, and experience with the system during the extensive coal combustion tests has been very favorable.

The heart of the coal feeding system is a Vibra-Screw Live Bin Feeder which is capable of feeding coal to 10 psig over a range of 4 to 40 lb/hr. The feeder bin capacity is 120 pounds. The coal feed rate is controlled and monitored via the simple system shown in Fig. 13. The feeder speed adjustment is operated by a reversible servo motor. An iron gear placed on the main feeder shaft rotates past a magnetic pickup located in close proximity to it. The pickup sends a signal to a frequency counter in the control room, providing a digital readout directly proportional to feeder speed.

Coal is emptied from the bottom of the bin by a hollow feed screw as shown in Fig. 13. The feed screw causes pulsations in the coal feed rate that in turn would cause flame instabilities if allowed to persist.

Figure 13. Feeder Control/Monitoring Schematic (George et al., 1977)

The entrainment vessel, illustrated in Fig. 14, was designed to smooth out these pulsations. The vessel is connected to the feeder by a flexible hose and is vibrated by a magnetic vibrator at its base (Erietz Magnetics, Inc.). Coal particles fall onto the sloping wooden cone and gradually fall off the edge into the bottom of the vessel, where they are entrained by swirling primary air and carried out the bottom. The reduction in magnitude of the oscillations is considerable, and no flame instabilities have been observed.

The calibration of the coal feeder under entrained conditions is presented in Fig. 15. Each data point represents a run of six minutes' duration and was made by catching the coal particles in a bag filter. A parabolic fit to the points of Fig. 15 is used in the data reduction program to calculate coal feed rates (Appendix B).

3. Product Gas Sampling and Analysis

Figure 16 is a schematic diagram of the product gas sampling system. A stainless steel water-cooled probe is used to draw a sample from the reactor exhaust. A ceramic fiber filter attached to the probe tip 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. The UTI Q-30C quadrupole mass spectrometer (Uthe Technology International, Inc.) is calibrated for the seven gases of interest (N_2 , O_2 , H_2O , CO_2 , H_2 , CO , CH_4). Water vapor can be sampled directly due to a heated inlet system. 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) and George et al. (1977).

Figure 14. Coal Entrainment Vessel (George, 1978)

Figure 15. Coal Feeder Calibration

Figure 16. Sampling System Schematic
(George et al., 1977)

IV. MACROSCOPIC MODEL FOR THE PULVERIZED COAL CYCLONE REACTOR

The cyclone model of Thomas (1978) described in Chapter II has been improved and expanded. The significant new features include (1) a pyrolysis model in which the volatiles yield is a function of reactor temperature and pyrolysis zone residence time; (2) a check of the model kinetics against the limitations imposed by gas-phase equilibrium and (3) the ability to model fuel-rich gasification via stoichiometric limitations on the amount of carbon reacted and gas-phase equilibrium to determine product gas composition. The cyclone model with all the new features included will hereafter be referred to as the revised Thomas model. In the discussion to follow emphasis is on the new features of the model; the original framework will be discussed briefly with frequent reference to Thomas (1978).

The major input and output variables for the model are those used in the experiment. Primary and secondary air flowrates and temperatures, coal composition and size distribution, and reactor geometry are input variables. The major output variables include the product gas composition and temperature and carbon efficiency; gasification parameters (heating value, cold and hot gas efficiencies, make gas yield and combustible make gas yield) are calculated for fuel-rich runs. The fundamental structure of the model remains as illustrated in Fig. 4. The revised assumptions are summarized in Table 7.

A. Pyrolysis Zone

Incoming coal particles are assumed to follow a Rosin-Rammler size distribution as recommended by Field et al. (1967) and expressed as

Table 7. Revised Thomas 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 formed.
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 (CO_2 is only formed in the gas-phase reaction) 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 7. (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.

$$RR = 100 \exp[-(d/\bar{d})^x] \quad (4-1)$$

where d is the particle diameter (μm), RR the weight percent of coal of a size greater than d , and $\bar{d}$ and x are measures of average size and size dispersion, respectively. Values suggested by Field et al. (1967) are $\bar{d} = 53$ microns and $x = 1.2$; the distribution for the pulverized coal used in the experiments is virtually identical, with $\bar{d} = 56$ microns and $x = 1.23$ (George et al., 1977). A minor improvement over the Thomas model is that the particles need not be moisture-free.

The incoming coal-air mixture enters the pyrolysis zone at high velocity. Due to 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 the following energy balance:

$$\begin{aligned} &(\text{rate of heat transfer to the particle by radiation}) + \\ &(\text{rate of heat transfer to the particle by convection}) = \\ &(\text{rate of change of particle internal energy}) \end{aligned} \quad (4-2)$$

Radiant heat transfer is calculated by assuming that the particle is spherical and is surrounded by two infinite planes, one at the flame temperature T_f and one at the wall temperature T_w where $T_w = T_f - 50^\circ\text{R}$ from previous model runs. The resulting expression for radiative heat transfer to the particle $Q_{p,r}$ (BTU/hr) is (Holman, 1972)

$$Q_{p,r} = A_p \epsilon_p \sigma (.5 T_f^4 + .5 T_w^4 - T_p^4) \quad (4-3)$$

where A_p is the particle area (ft^2), ϵ_p the particle emissivity, σ the Stefan-Boltzmann constant ($\text{BTU/hr-ft}^2\text{-}^\circ\text{R}^4$) and T_p the particle temperature ($^\circ\text{R}$). A value of $\epsilon_p = 1.0$ was used as suggested by Field et al. (1967).

Heat transfer by convection is expressed as (Holman, 1972)

$$Q_{p,c} = A_p h (T_f - T_p) \quad (4-4)$$

where h is the convection coefficient ($\text{BTU/hr-ft}^2\text{-}^\circ\text{R}$), calculated as follows:

$$h = \text{Nu}_f k_g / d \quad (4-5)$$

where Nu_f is the Nusselt number, k_g the gas thermal conductivity ($\text{BTU/hr-ft-}^\circ\text{R}$) and d the particle diameter (ft). A value of $\text{Nu}_f = 4.0$ was used as suggested by Field et al. (1967). Gas thermal conductivity was calculated via a linear fit to tabulated air data (Vargaftik, 1975). Badzioch and Hawksley (1970) conducted tests with closely size-graded particles and found no significant effect of particle size on volatiles yield; thus the particle diameter for all heat transfer calculations was taken to be the mass average value.

The rate of change of particle temperature is thus simply calculated as

$$Q_{p,r} + Q_{p,c} = 3600 (\rho \pi d^3 / 6) c_p dT_p / dt \quad (4-6)$$

where ρ is the particle density (lb/ft^3), c_p the specific heat ($\text{BTU/lb-}^\circ\text{R}$) and t the time (sec). A value of $c_p = .3 \text{ BTU/lb-}^\circ\text{R}$ is used as suggested by Smoot and Horton (1977). Eqn. (4-6) is integrated numerically to yield particle temperature as a function of time. Particle heating rates are in the range of 10^5 to 10^6 $^\circ\text{R/sec}$ and are comparable to those cited in the literature for pulverized coal flames (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. 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 (see Section II.D). The overall expression derived by Kobayashi et al. (1977) for the coal mass fraction volatilized is

$$f_v = \int_0^t (\alpha_1 k_1 + \alpha_2 k_2) \exp\left[-\int_0^t (k_1 + k_2) dt\right] dt, \quad (4-7)$$

$$k_1 = B_1 \exp(-E_1/RT_p) \quad (4-8)$$

$$k_2 = B_2 \exp(-E_2/RT_p) \quad (4-9)$$

where α_1 and α_2 are mass stoichiometric coefficients, B_1 and B_2 frequency factors (sec^{-1}), E_1 and E_2 activation energies (kcal/g-mole), R is the universal gas constant ($\text{kcal/g-mole}^\circ\text{K}$) and T_p the particle temperature ($^\circ\text{K}$). 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, on a dry ash-free basis. In order to model the pyrolysis of a coal with significant moisture content it is necessary to modify the mass stoichiometric coefficients to account for the evolution of water vapor. Solomon (1977) found that moisture is typically evolved at low temperatures; thus α_1 and α_2 are modified as

$$\alpha_{1,m} = \alpha_1 (1 - f_{\text{ASH}} - f_{\text{H}_2\text{O}}) + f_{\text{H}_2\text{O}} \quad (4-10)$$

$$\alpha_{2,m} = \alpha_2 (1 - f_{\text{ASH}} - f_{\text{H}_2\text{O}}) \quad (4-11)$$

where $\alpha_{1,m}$ and $\alpha_{2,m}$ are mass stoichiometric coefficients on an as-received basis and f_{ASH} and $f_{\text{H}_2\text{O}}$ are the coal ash and moisture mass fractions.

A closed form solution to Eqn. (4-7) is obtained by assuming a constant particle temperature; yields are thus calculated for the model in a stepwise isothermal fashion. The particle weight loss curves, when

converted to a dry ash-free basis, agree very closely with the theoretical curves (see Fig. 10) of Kobayashi et al. (1977).

Figure 10 shows that for moderate gas temperatures (1500°K) coal particles may require as much as 150 msec 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 reactor temperatures of 1500°K (typical of gasification conditions) the pyrolysis yield is then limited by particle residence time for air flowrates of 125 lb/hr and greater. This is particularly significant since carbon efficiency and product gas composition under gasification conditions are enhanced by high air flowrates (see Section V.E). Under combustion conditions the effect of residence time is minimal due to the higher temperatures and more rapid pyrolysis rates.

All of the coal H, N, O, S and moisture is assumed to pyrolyze based on the findings of Solomon (1977). For very low temperature trials, the mass fraction volatilized is sometimes less than the combined mass fractions of the above constituents; when this occurs the mass fraction volatilized is arbitrarily increased to include all the H, N, O, S and moisture for compatibility with the rest of the model. Volatiles burn instantaneously forming H₂O, NO, SO₂ and CO.

The heat released by volatiles combustion is calculated by assuming that the pyrolysis process is thermally neutral (Kobayashi et al., 1977) and that the carbon remaining in the char is amorphous with a heating value Q_C of 14110 BTU/lb. An energy balance for the heat released due to volatiles combustion thus yields

$$\dot{Q}_V = \dot{m}_{\text{coal}} Q_{\text{coal}} - \dot{m}_{\text{char}} \omega_C Q_C - F_{\text{CO}} Q_{\text{CO}} \quad (4-12)$$

where $\dot{Q}_V$ is the heat release (BTU/lb), $\dot{m}_{\text{coal}}$ the coal feed rate (lb/hr), Q_{coal} the lower heating value of coal (BTU/hr), $\dot{m}_{\text{char}}$ the flowrate of char leaving the pyrolysis zone (lb/hr), ω_C the char carbon mass fraction, F_{CO} the CO flowrate leaving the pyrolysis zone (lbmole/hr) and Q_{CO} the heat of combustion of CO (BTU/lbmole). F_{CO} , $\dot{m}_{\text{char}}$ and ω_C are given by Eqns. (4-15), (4-18) and (4-22), respectively.

Based on the preceding analysis, the flowrates of gaseous species and char from the pyrolysis zone can be calculated as follows (Thomas, 1978):

$$F_{H_2O} = \dot{m}_{coal} f_H/2 + \dot{m}_{coal} f_{H_2O} \quad (4-13)$$

$$F_{NO} = \dot{m}_{coal} f_N/14 \quad (4-14)$$

$$F_{CO} = \dot{m}_{coal} f_{C,v}/12 \quad (4-15)$$

$$F_{SO_2} = \dot{m}_{coal} f_S/32 \quad (4-16)$$

$$F_{O_2} = F_{O_2,i} - \frac{1}{2}(\dot{m}_{coal} f_H/2 + F_{NO} + F_{CO}) - F_{SO_2} + \dot{m}_{coal} f_O/32 \quad (4-17)$$

$$\dot{m}_{char} = \dot{m}_{coal} (1 - f_v) \quad (4-18)$$

and

$$f_{C,v} = f_v - f_H - f_N - f_O - f_S - f_{H_2O} \quad (4-19)$$

where F_{H_2O} , F_{NO} , F_{CO} , F_{SO_2} and F_{O_2} are the gaseous species flowrates (lbmole/hr), $\dot{m}_{char}$ the char flowrate (lb/hr), $\dot{m}_{coal}$ the coal feed rate (lb/hr), f_H , f_{H_2O} , f_N , f_S and f_O the coal mass fractions of the indicated species, and $f_{C,v}$ the fraction of the coal carbon released with the volatiles. $F_{O_2,i}$ is known from the incoming air flowrate, as is $F_{N_2,i}$ which is constant throughout the reactor.

Bituminous coals are known to swell during pyrolysis. Essenhigh (1977) suggests a diameter increase of 10% to simulate swelling. With this in mind, the size, density and carbon mass fraction of the char particles leaving the pyrolysis zone are (Thomas, 1978)

$$a_c = s a_{coal} \quad (4-20)$$

$$\rho_c = \rho(1 - f_v)/s^3 \quad (4-21)$$

$$\omega_c = (f_c - f_{c,v})/(1 - f_v) \quad (4-22)$$

where a_c is the char particle radius, s the swelling factor (1.1), a_{coal} the coal particle radius, ρ and ρ_c the particle densities before and after pyrolysis, ω_c the char carbon mass fraction and f_c the coal carbon mass fraction.

B. PSR Zone

1. Particle Behavior and Homogeneous Kinetics

The PSR zone of the Thomas model was discussed in some detail in Chapter II. Recall that char particles burn in the PSR until they reach a critical size determined by a force balance analysis. Char carbon burns to form CO, which in turn may burn in the gas phase; thus two reactions occur in the PSR zone (Thomas, 1978):

and

The rate of Eqn. (4-23) is calculated from a mass balance of particles entering and leaving the PSR zone, expressed as (Thomas, 1978)

$$r_c V_{\text{PSR}} = \frac{\omega_c}{12} \left[\sum_{j=1}^n \frac{4}{3} \pi \rho_c N_j r_j^3 + \sum_{j=n+1}^{\infty} \frac{4}{3} \pi \rho_c N_j (r_j^3 - a^3) \right] \quad (4-25)$$

where $r_c V_{\text{PSR}}$ is the char carbon oxidation rate (lb-moles/hr), ω_c is defined by Eqn. (4-22), ρ_c by Eqn. (4-21), a is the critical particle radius (ft),

$r_j \leq a$ for $j \leq n$ and $r_j > a$ for $j > n$, and N_j is the number flowrate of particles of radius r_j . The first term in Eqn. (4-25) accounts for particles whose radii are smaller than the critical radius which burn completely in the PSR; the second term accounts for larger particles which burn until they reach the critical radius, at which point they enter the PFR.

The rate at which CO is converted to CO₂ is calculated via Eqn. (2-3). For a perfectly stirred reactor operating at steady state, the chemical reaction rates are constant and the exit conditions (species concentrations and temperature) are equal to those in the reaction chamber; thus the flowrate of CO leaving the PSR, $F_{CO,o}$ (lbmole/hr), can be calculated by species conservation (Smith, 1970):

$$F_{CO,o} = F_{CO,i} + r_C V_{PSR} - r_{CO} V_{PSR} \quad (4-26)$$

where $F_{CO,i}$ is the CO flowrate into the PSR zone (lbmole/hr), $r_C V_{PSR}$ is defined by Eqn. (4-25) and r_{CO} by Eqn. (2-3). The flowrates of other gaseous species leaving the PSR zone are calculated via simple mass balances (Thomas, 1978).

2. Stoichiometric Limitations

The analysis cannot proceed as indicated above if insufficient oxygen exists to convert all the char carbon released via Eqn. (4-25) to CO; this occurs when

$$2 F_{O_2,i} < r_C V_{PSR} \quad (4-27)$$

where here $F_{O_2,i}$ is the oxygen flowrate into the PSR zone (lbmole/hr). For the coals used on this project, this limitation corresponds to an air/fuel ratio of approximately 55 percent of stoichiometric. For air/fuel ratios below this point, the char oxidation rate is calculated as

$$r_C V_{PSR} = 2F_{O_2,i} \quad (4-28)$$

The outlet flowrates of CO, CO₂, O₂, H₂ and H₂O are then determined through C, H and O balances and two chemical equilibria via the following equations:

$$F_{CO,i} + r_C V_{PSR} = F_{CO,o} + F_{CO_2,o} \quad (4-29)$$

$$F_{H_2O,i} = F_{H_2,o} + F_{H_2O,o} \quad (4-30)$$

$$F_{CO,i} + F_{H_2O,i} + 2 F_{O_2,i} = F_{CO,o} + F_{H_2O,o} \quad (4-31)$$

$$+ 2 F_{CO_2,o} + 2 F_{O_2,o}$$

$$K_{p1} = \frac{F_{CO,o} F_{O_2,o}^{\frac{1}{2}}}{F_{CO_2,o}} \left[\frac{P}{F_{CO,o} + F_{CO_2,o} + F_{H_2,o} + F_{H_2O,o} + F_{NO,o} + F_{N_2,o} + F_{O_2,o} + F_{SO_2,o}} \right]^{\frac{1}{2}} \quad (4-32)$$

$$K_{p2} = \frac{F_{CO,o} F_{H_2O,o}}{F_{CO_2,o} F_{H_2,o}} \quad (4-33)$$

where $F_{m,i}$ and $F_{m,o}$ are flowrates of species m into and out of the PSR zone (lbmole/hr), P is the total pressure (1 atm), and K_{p1} and K_{p2} are equilibrium constants based on partial pressures. In this case, the outlet flowrate of O₂ is zero by virtue of Eqn. (4-28) and the flowrates of N₂, NO and SO₂ are unchanged from the exit of the pyrolysis zone. The equilibrium constants are evaluated via curve fits to the JANAF Table data given by Wark (1971). Once the molar flowrates of the gaseous species are known, the calculation of carbon efficiency and the gasification parameters is carried out as illustrated in Appendix B.

To summarize up to this point, coal particles enter the pyrolysis zone and are rapidly devolatilized by intense heating due to radiation

and convection. The volatile products instantly burn, forming H_2O , CO , NO and SO_2 . These constituents plus the char, N_2 and remaining O_2 then enter the PSR zone. 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 and all hydrogen remains in the form of H_2O ; in the latter case, the PSR gas composition is determined by chemical equilibrium. It remains to calculate the PSR temperature (in the nonisothermal case) and to check the PSR results against equilibrium considerations.

3. PSR Temperature and Equilibrium Checks

For the nonisothermal case, the PSR temperature is found from an energy balance (Thomas, 1978):

$$\sum_j \int_{T_{r,j}}^{T_f} \dot{m}_j c_{p,j} dT = \dot{Q}_{chem} - \dot{Q}_{loss} \quad (4-34)$$

$$\dot{Q}_{chem} = r_C V_{PSR} (12 Q_C - Q_{CO}) + r_{CO} V_{PSR} Q_{CO} + \dot{Q}_V \quad (4-35)$$

where $T_{r,j}$ are the initial reactant temperatures ($^{\circ}R$), T_f is PSR zone temperature ($^{\circ}R$), $c_{p,j}$ the specific heat of constituent j (BTU/lb $^{\circ}R$), $\dot{m}_j$ the mass flowrate of species j (lb/hr), $r_C V_{PSR}$ the rate of char oxidation (lbmole/hr), $r_{CO} V_{PSR}$ the rate of CO oxidation (lbmole/hr), Q_C and Q_{CO} are the heats of combustion of amorphous carbon (BTU/lb) and CO (BTU/lbmole), $\dot{Q}_V$ is defined by Eqn. (4-12) and $\dot{Q}_{loss}$ is the reactor heat loss (BTU/hr), to be discussed shortly.

The calculated flame temperature is a convenient parameter for checking the kinetic results against the limitations imposed by equilibrium. The equilibrium analysis consists of the simultaneous solution of Eqns. (4-29) through (4-35) by an iterative method. The kinetically determined flowrates and temperature are used as initial guesses. The temperature from the kinetic analysis is then compared to that obtained from the equilibrium model: if the kinetic temperature is higher, the

results are in violation of the second law and the equilibrium solution is the correct one. Typically, the kinetic and equilibrium temperatures are within 10^0R of each other for both fuel-rich and fuel-lean cases.

For the isothermal case, flame temperature is fixed and the H_2 molar flowrate is assumed to be zero. Thus the only parameter available for comparison between the kinetic and equilibrium analyses is the CO/CO_2 ratio. The equilibrium analysis is reduced to Eqns. (4-29) through (4-33) since the temperature is known. The results of the kinetic analysis are considered invalid if the kinetic CO/CO_2 ratio is less than the equilibrium CO/CO_2 ratio; the equilibrium condition is then used for calculating the PSR zone outlet flowrates.

When oxygen is depleted in the PSR during fuel-rich runs, the conversion of CO to CO_2 is halted and the species flowrates are "frozen" at that point. However, this situation is not realistic because other mechanisms are available to carry the system toward equilibrium. To remedy this situation, the gas-phase constituents are assumed to go to equilibrium when oxygen is depleted. Results of Elliott et al. (1952) and the present investigation (Chapter V) show that the gas-phase composition is reasonably close to equilibrium for fuel-rich cases.

4. Reactor Heat Loss

Thomas (1978) developed a detailed heat loss model for the cyclone in which heat transfer is examined in three portions: (1) convection and radiation to the chamber walls and through wall openings; (2) conduction through the reactor walls, insulation and pressure vessel and (3) radiation and free convection from the vessel to the surroundings.

Convection heat transfer to the chamber walls was included because of the high gas velocities characteristic of cyclones. Since heat transfer correlations for swirling flows are not readily available, the walls, roof and floor of the cyclone were treated as flat plates, a technique also used by Lewellen et al. (1977). Since wall curvature is known to enhance heat transfer, a high characteristic gas velocity was purposely chosen. The resulting heat transfer coefficient was compared

to one based on a turbulent pipe flow analysis: the results were nearly identical.

Radiation heat transfer from the flame to the walls was calculated by treating the two as concentric gray cylinders with emissivities of .6 and .7, respectively (Thomas, 1978). For radiation from the flame to the slag tap and throat tube, the ports were treated as concave surfaces completely surrounded by the flame. The above three avenues of heat transfer inside the chamber were found to be of the same order of magnitude, indicating that each contributed significantly to the overall heat loss.

Conduction heat transfer was calculated by modeling the reaction chamber, insulation and pressure vessel as concentric spheres (Krieth, 1965). Such a method is appropriate for small, heavily insulated cavities. Radiation heat transfer from the pressure vessel was calculated by assuming that the surrounding room acted as a blackbody. The free convection model was slightly more difficult, involving separate correlations for the top, sides and bottom of the vessel. The full details of the cyclone heat loss model are presented by Thomas (1978); typical theoretical reactor heat losses are 10 to 15 percent, with corresponding experimental values of 20 to 25 percent.

C. PFR Zone

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 volume of the PFR zone is given by (Thomas, 1978)

$$V_{PFR} = \pi R_t^2 (L - L_t + l_t) \quad (4-36)$$

with the open and enclosed portions given by

$$V_{PFR,1} = \pi R_t^2 (L - L_t) \quad (4-37)$$

and

$$V_{PFR,2} = \pi R_t^2 l_t \quad (4-38)$$

where R_t is the throat tube radius (ft), L the chamber length (ft), L_t the throat tube length (ft) and l_t is defined in Fig. 5. The PFR zone is divided into approximately 300 discrete increments to insure calculation accuracy.

Calculations within each increment of the PFR proceed as follows. The flow of constituent y into the j^{th} volume increment is expressed as (Thomas, 1978)

$$F_{y,i,j} = F_{y,o,j-1} + \frac{\Delta V_{PFR,j} F_{y,PSR}}{V_{PFR,1}} \cdot X \quad (4-39)$$

where $X = 1$ for a volume increment $\Delta V_{PFR,j}$ within $V_{PFR,1}$ and $X = 0$ for a volume increment within $V_{PFR,2}$. $F_{y,i,j}$ is the flow of y into $\Delta V_{PFR,j}$ (lbmole/hr), $F_{y,o,j-1}$ the flow out of $\Delta V_{PFR,j-1}$ (lbmole/hr), and $F_{y,PSR}$ the flow of y leaving the PSR zone (lbmole/hr).

The carbon monoxide and char oxidation rates are calculated via Eqns. (2-3) through (2-6). The concentrations and temperature required for these kinetic expressions are based on the incoming molar flowrates and temperature. The oxidation of char in the PFR takes place under combined kinetic and diffusion control (Eqn. 2-4); recall that in the PSR, the extent of char conversion was controlled by the force balance treatment.

The char and gaseous species flowrates leaving the increment are calculated by simple species conservation equations (Thomas, 1978). For the nonisothermal case, the energy equation is used to find the increment temperature, just as it was in the PSR, except that no heat losses

are considered from the PFR zone. The results of the kinetic analysis are checked against equilibrium results in exactly the same fashion as was used in the PSR zone. At the end of the PFR zone the carbon efficiency (and gasification parameters for fuel-rich runs) are calculated as shown in Appendix B using the appropriate product gas composition, i.e., kinetic or equilibrium, depending on the outcome of the check.

D. Model Results and Discussion

The important results of the Thomas model were presented in Chapter II. In this section, comparisons are made between the Thomas model and the revised model (the original model plus the pyrolysis and equilibrium calculations). Model runs were made with a dry Southern Indiana bituminous coal (Appendix C); further parameters are given in Table 8.

Figure 17 displays the molar CO/CO_2 ratio in the PSR zone as a function of temperature, air flowrate and stoichiometry for both the kinetic and equilibrium analyses. The isothermal version of the model was used, and the revised pyrolysis model was left out so that the total amount of carbon present in the gas phase ($\text{CO} + \text{CO}_2$) would be the same for both cases.

For stoichiometric mixtures the amount of CO present at equilibrium is negligible for the range of temperatures considered, as one might expect. For the fuel-rich case the equilibrium ratio is a function of both flowrate and temperature. Increased flowrate increases the carbon efficiency due to enhanced centrifugal effects; thus the equilibrium CO/CO_2 ratio increases because the gas-phase oxygen concentration decreases (see Eqn. (4-32)). The effect of temperature is twofold: (1) increased temperature also enhances centrifugal effects by increasing the volumetric flowrate for a given mass flowrate; thus the equilibrium CO/CO_2 ratio increases for the reason stated above and (2) dissociation of CO_2 to CO and O_2 increases with temperature.

The kinetic CO/CO_2 ratios increase with air flowrate due to decreased gas residence time. Increasing temperature produces two opposing effects: (1) conversion of CO to CO_2 is enhanced by more rapid

Table 8. Parameter Values Used for Model Calculations

<u>Quantity</u>	<u>Symbol</u>	<u>Value</u>
Cyclone Geometry		
Chamber Length	L	.833 ft
Chamber Radius	R ₁	.250 ft
Throat Tube Length	L _t	.167 ft
Throat Tube Radius	R _t	.0729 ft
Throat Tube Length Plus Uncooled Portion of Exhaust	ℓ _t	.542 ft
Emissivities		
Pressure Vessel Emissivity	ε _v	.8
Flame Emissivity	ε _f	.6
Chamber Wall Emissivity	ε _w	.7
Particle Emissivity	ε _p	1.
Coal Properties		
Density	ρ	85 lb/ft ³
Specific Heat	c _p	.3 BTU/lb-OR
Average Particle Size	d̄	53 μm
Rosin-Rammler Dispersion Factor	x	1.2
Heating Value	Q _{coal}	11460 BTU/lb
Pyrolysis Parameters		
Swelling Index	s	1.1
Mass Stoichiometric Coefficients	α ₁	.3
	α ₂	1.
Frequency Factors	B ₁	2 x 10 ⁵ s ⁻¹
	B ₂	1.3 x 10 ⁷ s ⁻¹
Activation Energies	E ₁	25 kcal/gmole
	E ₂	40 kcal/gmole
Carbon Monoxide Kinetics		
Frequency Factor	k ₀	1.3 x 10 ¹⁴ cm ³ /gmole-s
Activation Energy	E	30 kcal/gmole
Char Kinetics		
Frequency Factor	A	8 g/cm ² -s-atm
Activation Energy	E	16 kcal/gmole

Figure 17. Molar Ratio of CO/CO₂ in the PSR Zone as a Function of Flame Temperature, Air Flowrate and Stoichiometry

kinetics and (2) gas residence time decreases due to higher volumetric flowrate. The kinetic effect apparently dominates since the kinetic CO/CO_2 ratios decrease substantially with temperature, particularly below 2400°R .

A comparison between the kinetic and equilibrium curves reveals that kinetic effects in the PSR are important, particularly at low flame temperatures. Even as temperature increases above 2400°R , the kinetic CO/CO_2 ratio is significantly higher than the equilibrium ratio for the fuel-rich case. These findings are in agreement with the results of Kalishevskii and Ganchev (1967) who found significant CO concentrations within a coal burning cyclone. The results suggest that product gas heating value can be enhanced by operating at relatively low reactor temperatures and high gas throughputs to take advantage of the observed departure from equilibrium.

Figure 18 displays the carbon efficiency as a function of temperature, air flowrate and stoichiometry for the isothermal case of both the original and revised models. The effects of flowrate and stoichiometry on carbon efficiency were discussed in detail for the original model in Chapter II; since the same trends are evident for the revised model these effects will not be discussed further. The most important feature shown in Fig. 18 is the much stronger effect of temperature on carbon efficiency for the revised model as compared to the original model. A comparison of PSR zone carbon efficiencies shows that the pyrolysis model is responsible for virtually all of this difference. Recall that for a given flowrate the particle size leaving the PSR zone is determined by the force balance. However, the particle composition (mass fractions of ash and carbon) depends on the amount of carbon pyrolyzed since particle composition is unchanged after the pyrolysis stage. In the revised model, the amount of carbon pyrolyzed and thus carbon efficiency is a strong increasing function of temperature. Hence, carbon efficiency predicted by the revised model is less than the original version at lower temperatures and greater than the original at higher temperatures.

Figure 18. Carbon Efficiency as a Function of Flame Temperature, Air Flowrate and Stoichiometry for the Original and Revised Models

Carbon efficiency was essentially unaffected when the kinetic results were replaced with the equilibrium results. At low temperatures (2000-2400^oR) where the kinetics are slow, the kinetic results were very seldom in violation of the second law. At high temperatures (3200-3600^oR), however, the kinetic conversion of CO to CO₂ was consistently too complete and the equilibrium molar flowrates were used.

In Fig. 19 the carbon efficiencies and exit temperatures predicted by the original and revised models are plotted as functions of stoichiometry for the nonisothermal case. The air flowrate for all runs is 200 lb/hr. The most important feature of the temperature profiles is that the equilibrium treatment in the revised model failed to reduce the exit temperatures substantially. Only on the fuel-rich side of stoichiometric were significant numbers of second law violations observed; the typical magnitude of such violations was 5 to 20^oR. For all other conditions the kinetic and equilibrium temperatures were virtually identical. A check of CO/CO₂ ratios (the criterion used in the isothermal case) showed generally good agreement with the temperature criterion; in those instances where the two criteria disagreed (stoichiometric and slightly air-rich cases) the amount of CO present was so slight as to have a minimal impact on the gas temperature. The higher temperature near stoichiometric conditions for the revised model is due to the increase in carbon efficiency resulting from the revised pyrolysis treatment.

The original and revised carbon efficiency profiles are similar to the temperature profiles in that they exhibit a broad peak on the air-rich side. Carbon efficiency in the revised model increases at higher temperature (Fig. 18) and also increases somewhat with air/fuel ratio; thus the peak in carbon efficiency is at nearly the same stoichiometry as the peak in temperature. Carbon efficiency in the original model is a weaker function of temperature and thus peaks at a slightly higher air/fuel ratio due to the effect of stoichiometry.

Carbon efficiency as calculated with the revised model is higher than the corresponding value from the original model for most of the range indicated due to the high reactor temperatures and the corresponding effect on the amount of carbon pyrolyzed. The two carbon efficiencies

Figure 19. Carbon Efficiency and Gas Exit Temperature as Calculated with the Original and Revised Models (Air Flowrate: 200 lb/hr)

are equal when the exit temperature is roughly 2800°R ; at this temperature the coal mass fraction volatilized as predicted by the revised model is .430, which compares closely with the constant volatiles fraction of .40 used in the original model. Thus the observed trends in carbon efficiency are readily explained by the changes made in the model; however, the range of values encountered is so narrow that experimental confirmation of the theoretical trends is doubtful.

In summary, the gross reactor behavior predicted by the revised model is not substantially different from the behavior predicted by the original Thomas model. The effect of temperature on carbon efficiency is greater as a result of the temperature-dependent pyrolysis yield; however, the range of values predicted is still so narrow that the trends are likely to be masked by experimental scatter. The comparison of the kinetic molar flowrates and temperatures with the limitations imposed by equilibrium revealed that the kinetic results were often in violation of the second law; however correcting the violations by reverting to equilibrium values had little impact on overall reactor behavior. The most significant improvement in the revised model is the capacity to model fuel-rich gasification via the stoichiometric limitations imposed on the amount of char oxidized in the PSR (Section B.2). The importance of this feature will be demonstrated in Chapter V where the predictions of the macroscopic model are compared with the experimental results from the cyclone reactor.

V. EXPERIMENTAL RESULTS AND COMPARISON WITH THEORY

A broad range of experiments has been completed in the cyclone since testing began in September, 1977. The first two series of tests were methane combustion tests, conducted to observe the reactor under clean combustion conditions. After typical startup problems were corrected, sufficient methane trials were run to provide confidence in the integrity of the system and in the quality of the experimental results. Initial coal combustion tests were also far from trouble-free; however the difficulties were overcome and three series of coal combustion tests and one fuel-rich gasification test have been completed. A computerized data reduction program has been written to analyze the voluminous amount of data produced; the program is described briefly in this chapter and in detail in Appendix B.

The important results of the methane combustion tests and the early coal combustion tests will be presented briefly in this chapter. 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 percent for the 46 trials of series three and (2) stable operation to an equivalence ratio of 2.4 with a carbon efficiency of 77 percent in series four.

A. Data Reduction Program

The data reduction program is divided into three main sections to reduce data from methane combustion, coal combustion and coal gasification trials. The many subroutines that carry out the bulk of the calculations are summarized in Table 9. Three mass balance analyses are conducted by the program using the uncorrected product gas spectrum and two

Table 9. Data Reduction Program Subroutines

<u>Subroutine</u>	<u>Quantity (ies) Calculated</u>	<u>Method</u>
OFLO	flowrates of gases measured by orifices	standard equations from ASME Power Test Codes (1959)
AMGFLO	product gas flowrate	nitrogen gas used as an inert tracer; gas analysis provides molar ratios
BLNCE	hydrogen and oxygen mass balance errors	$(\text{input species flowrate} - \text{output species flowrate}) / \text{input species flowrate}$
TOTERR	total mass balance error	$(\text{total reactant flowrate} - \text{total output gas and solid flowrate}) / \text{total reactant flowrate}$
CRBERR	corrected product gas spectrum and corresponding carbon efficiency	hydrogen and oxygen mass balance errors forced to zero; new product gas analysis and flowrate calculated
DRY	corrected product gas spectrum	dry analysis; water vapor added to create perfect oxygen balance
CORECT	corrected product gas temperature at reactor exit	energy balance on the reactor exhaust thermocouple
COLFRM	coal enthalpy of formation	coal enthalpy of combustion equation (Wark, 1971)
HTLOSS	reactor percent heat loss	$(\text{absolute enthalpy of reactants} - \text{absolute enthalpy of products}) / \text{absolute enthalpy of reactants}$

corrected spectra generated within the program. The error indicators when using the uncorrected spectrum are the hydrogen and oxygen mass balance errors, expressed as

$$MBE = \frac{(\text{species input} - \text{species output})}{\text{species input}} \quad (5-1)$$

Typical magnitudes of the hydrogen and oxygen mass balance errors during coal trials are 36 and 8 percent, respectively, clearly demonstrating the need for further analysis. Most of the observed errors are due to difficulties in sampling for water vapor.

A corrected product gas spectrum is generated by forcing the hydrogen and oxygen mass balance errors to zero (see the description of subroutine CRBERR in Appendix B). Since the molar flowrates of all the product gas constituents (including the carbon-containing species) are altered by this method, a check on the sensitivity of carbon efficiency to the hydrogen and oxygen mass balance errors can be made. Typically the carbon efficiency calculated using the corrected spectrum is 5 percent less than that calculated from the original spectrum.

The third and most consistent method of data analysis makes use of the original spectrum on a dry basis to which enough water vapor has been added to create a perfect oxygen balance. Only the molar flowrate of water vapor is altered, so carbon efficiency is unaffected. The hydrogen mass balance error serves as a check on internal consistency; the average magnitude of 8.9 percent for the 67 trials of series 3 and 4 demonstrates the virtue of this approach which has been used to calculate all the data presented in this chapter except the first set of methane combustion data.

B. Methane Combustion Tests

The methane combustion experiments were an important first step in the cyclone experimental program. Important considerations such as ignitor stability, refractory integrity and sampling system reliability

were investigated during the early tests. More recently, methane flames were used to provide cyclone exhaust temperature and species profiles. Methane fires are more suitable than coal fires for such measurements due to their excellent stability. During all these tests methane was introduced to the cyclone via the torch ignitor.

Early methane tests were hampered by erratic ignitor operation and an inability to obtain reliable water vapor measurements. The ignitor instabilities were caused by the high temperature failure of a ceramic insulator; replacement with a quartz insulator solved the problem. Water vapor sampling problems were caused by the condensation and subsequent evaporation of water within the sampling system. Maintaining the probe and sampling lines at higher temperatures and scanning for a longer period for each mass spectrum improved the results; however, difficulties in sampling for water vapor were frequently encountered in later tests.

Results of methane combustion tests at a variety of stoichiometries are presented in Fig. 20. The uncorrected experimental mole fractions for methane flowrates of 35 and 45 g-moles/hr are compared with the equilibrium composition of a carbon-air-steam mixture at 1000°K , typical of reactor exhaust temperatures. The agreement between the experimental data and the equilibrium curves is very good, particularly for the air-rich cases. The discrepancy in the water vapor data on the fuel-rich side is of little concern since water vapor mole fractions on the order of 20 percent are not encountered in coal combustion or gasification tests. Carbon monoxide was detected by the mass spectrometer during the fuel-rich tests, but not in sufficient quantities to make reliable measurements. The CO readings presented in Fig. 20 were taken with an infrared CO analyzer. The significant result of this series of tests was the demonstrated ability of the mass spectrometer to resolve mixtures of gases produced and sampled under actual combustion conditions.

The cyclone exhaust was also traversed with a thermocouple and a velocity probe to determine the nature of the radial temperature and velocity profiles (Fig. 21). The traverses were conducted immediately above the exit plane of the reactor where the exhaust gas thermocouple is usually located (Fig. 12). The temperature traverse was conducted with a methane fire in the reactor; the velocity traverse was performed

Figure 20. Product Gas Composition of Methane Combustion Runs
(Barnhart et al., 1978)

Figure 21. Cyclone Exhaust Temperature and Velocity Profiles

under cold flow conditions due to probe limitations. Air flowrates were comparable to those under coal combustion conditions. The principal objective of the latter test was to determine a characteristic gas velocity in the vicinity of the thermocouple bead for use in the thermocouple energy balance (see section C.4 of Appendix B).

The axial velocity profile is highly nonuniform, exhibiting a sharp peak near the chamber wall and a broad, weak recirculation zone around the center. Such a profile is characteristic of highly swirled flows due to the radial pressure gradient created by the swirling gases (Syred and Beer, 1974). The temperature profile is also nonuniform, dropping off sharply near the cold walls and exhibiting a shallow depression near the centerline. The important conclusions to be drawn from these measurements are (1) the gas velocity in the vicinity of the thermocouple bead is very low and can be assumed stagnant for thermocouple heat transfer calculations and (2) heat loss via conduction from the bead is negligible due to the fairly flat temperature profile near the exhaust centerline. The shallow dip in the temperature profile at the centerline is due to two effects: (1) cold gases are recirculated into this region from the wall-adjacent area and (2) low gas velocities result in very poor convective heat transfer, increasing the impact of radiative heat losses to the cooling coil.

A species traverse of the cyclone exhaust was conducted in a separate experiment with an air-rich methane fire in the reactor. Prior to this test all gas sampling had been done via a stationary exhaust probe under the assumption that the exhaust composition was uniform; the object of the species traverse was to confirm that assumption.

Results of this test are presented in Fig. 22 in the form of species mole fractions at nine radial locations. In order to perform this traverse it was necessary to replace the cooling coil with a hollow refractory cylinder (simply an extension of the reactor throat tube, Fig. 12). The sampling probe was inserted into the exhaust line through the upper cooling coil penetration fitting and through a radial hole in the refractory liner. The only appreciable scatter in the data of Fig. 22 occurred with the first spectrum recorded; thus improper sampling

Figure 22. Cyclone Exhaust Species Profiles

technique is more likely the explanation than a nonuniform profile. The agreement among the rest of the data points is excellent, confirming the assumption of a uniform exhaust composition.

C. Preliminary Coal Combustion Tests

A summary of all cyclone coal combustion tests is presented in Table 10. The preliminary tests are the first and second series. The Indiana bituminous coal used in series one was supplied by the Purdue University Physical Plant. Two Montana subbituminous coals were used in the later tests; both varieties were provided by the Minnesota Power and Light Company. Coal analyses were performed by Commercial Testing and Engineering Co. and are presented in Appendix C. In all four series a trial or data point is based on one set of flow and temperature data and the average of two mass spectra taken concurrently.

1. Series One

Early coal combustion tests were characterized by low exhaust temperatures ($< 1000^{\circ}\text{C}$) that fluctuated as much as 200°C in a matter of minutes. Exhaust gas composition was observed to vary in much the same manner. The average carbon efficiency for the fifteen trials of series one was 95 percent; however, values ranging from 78 to 113 percent were observed, and hydrogen mass balances were generally poor. Thus the behavior of the cyclone in terms of stability and consistency of results left much to be desired.

Slagging conditions were achieved in spite of the low reactor temperatures, but the behavior of the slag was not satisfactory. The slag port was bridged over by the viscous slag, which eventually accumulated to a depth of $3/4$ inch in the bottom of the reactor. Molten slag was entrained by exiting gases and deposited on the throat tube, nearly closing it. An attempt to melt the slag with the reactor heaters and a hot methane fire proved unsuccessful.

All four reactor heaters had burnt out and required replacement. The stainless steel primary and secondary air feed tubes were extremely

Table 10. Coal Combustion Test Summary

<u>Series</u>	<u>Test Date(s)</u>	<u>No. of Trials</u>	<u>Coal Type</u>	<u>Stoichiometry Range</u> <u>$(A/F)/(A/F)_S$</u>	<u>Air Flow Range</u> <u>(lb/hr)</u>	<u>Coal Feed Rate Range</u> <u>(lb/hr)</u>
1	5-31-78 6-1-78 6-2-78	15	Indiana Bituminous	1.20-1.75	100-175	7.4-16
2	8-28-78 8-31-78	8	Montana Subbituminous	1.20-1.40	85-150	9.5-15
3	10-5-78 10-31-78	46	Montana Subbituminous	.820-1.50	60-220	10-20
4	12-21-78	21	Montana Subbituminous	.420-1.30	80-130	10-30

corroded and were replaced. The throat tube was ruined by slag but the other refractory sections suffered only inconsequential damage and were repaired. Further modifications were made during the next three month period to improve the likelihood of proper slagging; the slag port was enlarged, the heaters were moved to a lower level around the refractory and a longer throat tube was installed to force the hot gases into the lower part of the reactor.

2. Series Two

A Montana subbituminous coal from the Rosebud seam was used in the second series because of its slightly lower ash fusion temperature (Appendix C). Slag flow was improved but still not satisfactory; the slag port bridged over and molten slag was once again entrained by the exiting gases and deposited in the throat tube. The resulting increase in chamber pressure drove hot combustion gases into the reactor annulus, forcing an end to series two after only eight trials.

The average carbon efficiency for this short series was 96 percent. Reactor stability was much improved, and hydrogen mass balance errors were satisfactory (average magnitude of 12.6 percent). Thus, with the exception of the slagging problem, series two represented a significant improvement over series one.

D. Extended Coal Combustion Tests

A mixture of equal parts by weight of Rosebud and McKay subbituminous coals was used in series three to improve slag flow. The ash fluid temperature of such a mixture is 60°F lower than that of either of the two burned alone (Appendix C). Slag flow through the port was achieved but continued for only a few minutes before it bridged shut again. The rate of accumulation of slag in the throat tube was much lower, apparently due to the favorable ash characteristics. The series was interrupted briefly after six trials to unclog the throat tube and then proceeded smoothly for six hours, yielding by far the most comprehensive set of data to date. A tabulation of the raw and reduced data from the 46 trials of series three appears in Appendix D.

In Fig. 23 carbon efficiency is plotted as a function of stoichiometry (reciprocal of equivalence ratio) for three ranges of air flowrate. The six slashed (/) data points were taken before the brief outage to unclog the throat tube. Any effect of stoichiometry or air flowrate on carbon efficiency is masked by the scatter in the data. The average carbon efficiency is once again very high (96 percent) and the internal consistency of the data is excellent, as shown by the magnitude of the average hydrogen mass balance error (6.8 percent). A comparison of Figs. 23 and 20 reveals considerably more scatter under coal combustion conditions than during methane combustion. The observed scatter is due primarily to variations in coal composition and fluctuations in feed rate, and is comparable to that reported by Elliott et al. (1952).

Also plotted on Fig. 23 are the carbon efficiencies predicted by the revised model for air flowrates of 80, 125 and 185 lb/hr (solid curves). Model predictions were made with the isothermal version of the model using the average exhaust temperature of series three - 1500°C. The range of values predicted by the model is in very close agreement with the experimental results. Furthermore, the effects of flowrate and stoichiometry on carbon efficiency, as determined by both model and experiment, are minimal. This result confirms the dominating influence of the force balance for fuel-lean conditions as discussed in Section IV.D.

With the exception of the slagging problem, the performance of the cyclone reactor as a coal combustor was excellent. Carbon efficiency, the single most important performance indicator for a coal burner, was routinely high throughout all three series. Stability problems were encountered in only the first series, and may have been due to inadequate chamber preheating or other manifestations of operator inexperience. Neither stoichiometry nor flowrate had any apparent effect on the gross behavior of the reactor for the range of conditions considered thus far.

Although slagging difficulties occupied a great deal of time and were mentioned frequently in this chapter, their importance should not be overestimated. The operability of somewhat larger cyclones under slagging conditions has been amply demonstrated (Hoy et al., 1958; Joubert, 1978; Elliott et al., 1952). Yagi and Kunii (1957) operated a small cyclone (8" diameter, 13" height) with no slag tap, allowing the slag to accumulate during a test, as was done during series three. The

Figure 23. Series Three Experimental and Theoretical Carbon Efficiencies. The slashed (/) data points indicate the first six trials.

accumulation of slag is a nuisance, but in no way invalidates the results achieved or casts doubt on the potential usefulness of cyclones in industry; simple solutions to this problem for small cyclones will be discussed in Chapter VI.

E. Fuel-Rich Gasification Tests

The object of the fourth series of coal tests was to gasify coal without steam addition by proceeding systematically to lower and lower air/fuel ratios. The potential for coal gasification via fuel-rich combustion was demonstrated by investigators in West Germany who produced a gas with a heating value of 100 BTU/scf with a carbon efficiency of 95 percent at an equivalence ratio of 2.0 (Traenckner, 1953). Gasification via fuel-rich combustion is cited by Way (1974) as a potential source of fuel for MHD power cycles. Researchers at Pittsburgh Energy Research Center and at Combustion Engineering are also investigating gasification via fuel-rich combustion, although only limited data are available (Joubert, 1978; Laurendeau, 1979).

The results reported by Traenckner (1953) were enhanced considerably by capturing and recycling escaping char particles; the present investigation included no particle recycle. The results achieved are nevertheless very encouraging. A mixture of Rosebud and McKay subbituminous coals was once again used. The experimental data from series four are tabulated in Appendix D.

1. Carbon Efficiency

The experimental carbon efficiencies from series four are plotted versus stoichiometry for two air flowrate ranges in Fig. 24. The trials on the air-rich side were performed under very carefully controlled conditions as a test of repeatability; the results are satisfactory, particularly for the trials at $(A/F)/(A/F)_S = 1.3$. Carbon efficiency is high (above 90 percent) until $(A/F)/(A/F)_S$ equals about .55, at which point a smooth but steep decrease begins. The data is too sparse to observe any correlation between carbon efficiency and air flowrate.

Figure 24. Series Four Experimental and Theoretical Carbon Efficiencies

The solid curve in Fig. 24 represents the carbon efficiencies predicted by the revised mathematical model. Predictions for the two experimental air flow ranges were virtually identical. The agreement between the experimental data and the model predictions is very good, even under very fuel-rich conditions where the proximity to the rich blowoff limit provides a more severe test of the efficacy of the model; the predicted carbon efficiencies are only slightly lower than the experimental values for reasons to be discussed shortly.

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 $(A/F)/(A/F)_S = .55$. Char kinetics in the PFR have a minimal effect in this range, as demonstrated by the fact that carbon efficiency does not increase perceptibly with air/fuel ratio (recall the linear dependence of PFR char oxidation on O_2 concentration).

For stoichiometries below $(A/F)/(A/F)_S = .55$ the amount of oxygen in the PSR is insufficient to convert all the char carbon to CO; this limitation overrides the particle force balance treatment and more and more unburned carbon leaves the reactor as the air/fuel ratio is reduced. Steam and carbon dioxide are also capable of oxidizing char, but the rates of these reactions are much lower than that of char oxidation by oxygen (Chung and Smith, 1978); this factor was therefore not included in the present model. The results at very low air/fuel ratios might well improve, however, if these mechanisms are included in future modifications.

2. Coal Gasification Parameters

The results of series four were also analyzed in terms of commonly used gasification performance indicators (George et al., 1977). The methods used to calculate these parameters are presented in Appendix B.

The make gas yield (mass ratio of make gas to coal fed) and combustible make gas yield are plotted in Fig. 25 as functions of air/coal ratio. Solid curves once again represent the predictions of the cyclone mathematical model. The make gas yield increases linearly with air/coal

Figure 25. Make Gas Yield and Combustible Make Gas Yield Versus Air/Coal Ratio

ratio, while combustible make gas yield peaks at air/coal = 3.75 (approximately 50 percent of stoichiometric air). The agreement between experiment and model for the make gas yield is nearly perfect; model predictions of combustible yield are a little high, although the trend at low air/coal ratios is correct.

Make gas yield is a parameter of secondary importance and is a function of stoichiometry and carbon efficiency; in view of the good agreement between the experimental and theoretical carbon efficiencies, it is not surprising that the make gas yields also agree well. The combustible make gas yield is a measure of the mass of carbon monoxide and hydrogen produced since no methane was observed in the product gas. Because of the low molecular weight of H_2 , the mole fraction of carbon monoxide in the product gas is the principal factor in determining combustible make gas yield. The model product gas analysis is calculated via a simple equilibrium treatment, and the experimental mole fraction of carbon monoxide was found to be less than predicted by equilibrium. Thus the observed discrepancy between experiment and theory is due to the carbon monoxide content of the product gas. The drop in combustible make gas yield below air/coal = 3.75 corresponds to the reduced carbon efficiency in that range (Fig. 24).

The three most important performance indicators are plotted in Fig. 26 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 84 BTU/scf. The burnability of such a gas was demonstrated by Dahmen and Syred (1975) who burned "waste" gases with heating values as low as 37 BTU/scf in a swirling combustor over wide load limits. Heating values predicted by the mathematical 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.

The factors which determine the make gas heating value are the carbon monoxide and hydrogen mole fractions. These gases have nearly identical enthalpies of combustion and are the only combustible product gas constituents. Experimental and theoretical hydrogen mole fractions

Figure 26. Hot Gas Efficiency, Cold Gas Efficiency and Heating Value Versus Air/Coal Ratio

are in close agreement for values of air/coal down to 4.0; below this point the experimental values continue to increase while the theoretical values remain constant. Theoretical carbon monoxide mole fractions decrease sharply below air/coal = 4.0, while the experimental CO mole fractions continue to increase. Increased CO and H₂ mole fractions at low air/coal ratios are 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. 24.

Also plotted in Fig. 26 is the cold gas efficiency, defined to be that portion of the coal heating value present as chemical enthalpy in the product gas and conveniently calculated as

$$\eta_{cg} = Q Y / (\Delta H_{C,coal} \rho_g M) \quad (5-3)$$

where Q is the make gas heating value (BTU/scf), Y the make gas yield (lb make gas per lb coal), $\Delta H_{C,coal}$ the coal enthalpy of combustion (BTU/lb), ρ_g the gas density at STP (lbmole/ft³) and M the product gas molecular weight (lb/lbmole). Molar density ρ_g is the same for all gases, and the product gas molecular weight increases only slightly with air/coal ratio since the gas is mostly nitrogen; thus for a given coal, the cold gas efficiency is roughly proportional to the product of make gas heating value and make gas yield. Recall that make gas yield is an almost linear function of air/coal ratio (Fig. 25). Thus one would expect the ratio of cold gas efficiency to make gas heating value to increase in linear fashion with increasing air/coal ratio, a trend that both the experimental data and model predictions follow.

The third parameter plotted in Fig. 26 is the hot gas efficiency, which includes the change in sensible enthalpy between reactants and products as well as the change in chemical enthalpy. Hot gas efficiency is expressed as (Laurendeau and Waite, 1977)

$$\eta_{hg} = \eta_{cg} + \Delta H_{pr}/\Delta H_{C,coal} \quad (5-4)$$

where ΔH_{pr} is the difference in sensible enthalpy between reactants and products (BTU/lbcoal) and η_{cg} and $\Delta H_{C,coal}$ are as previously defined. Thus hot gas efficiency equals cold gas efficiency plus a term which is a strong function of temperature and air/coal ratio.

If the second term in Eqn. (5-4) increases with air/fuel ratio, the difference between hot and cold gas efficiency should also increase. This trend is especially clear for the theoretical results, which are based on the isothermal model at 2850°R. There is scatter in the experimental values for hot gas efficiency that is not present in the cold gas efficiency results due to trials in which the reactor temperature was substantially different from the average value; most noticeable is the data point at air/coal = 6.4 for which the reactor exit temperature was 3340°R. With the exception of this point, the comparison between experimental and theoretical hot gas efficiencies is very similar to that between the experimental and theoretical cold gas efficiencies as would be expected.

In summary, the data plotted in Fig. 26 demonstrate that a readily combustible gas can be produced in the cyclone reactor via fuel-rich gasification. Heating value, cold gas efficiency and hot gas efficiency are certainly acceptable for a first endeavor. The agreement between experiment and theory is good; the incorrect trend in heating value at low air/fuel ratio is evidently a consequence of ignoring steam-carbon reactions.

A further check on the consistency of the experimental data can be obtained by comparing the experimentally determined value of the water-gas shift equilibrium constant to the value based on the observed exit temperature (Fig. 27). The equilibrium constant as defined in Fig. 27 represents an endothermic reaction and thus increases with increasing temperature. 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. Furthermore, the greatest discrepancy occurs at the lowest temperatures where chemical reaction rates are lowest.

Figure 27. Experimental and Theoretical Values of the Water-Gas Equilibrium Constant

3. Comparison with Literature Results

The data reported by Traenckner (1953) for the Ruhrgas process are the only substantial results available for gasification via fuel-rich combustion in a cyclone reactor. The heating value reported by Traenckner is roughly 20 percent greater than the best achieved during the present investigation (100 versus 84 BTU/scf); however the carbon efficiency in the Ruhrgas process was increased from 80 to 95 percent through particle recycle. Under conditions of no particle recycle the heating value of the product gas would be expected to decrease; if the decrease in heating value is roughly proportional to the decrease in carbon efficiency, the results of the Ruhrgas process are very similar to those of the present investigation. 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. 24 and 26).

Perry et al. (1950) compare experimental values of the water-gas shift equilibrium constant to theoretical values as was done in Fig. 27; their correlation shows similar agreement. For the same system Elliott et al. (1952) plot $\text{CO} + \text{H}_2$ yield as a function of oxygen to coal ratio and observe a broad peak at roughly 40 percent of stoichiometric oxygen flow. The best results in the present investigation were achieved at 50 percent of stoichiometric air; however, Elliott et al. fed steam at the rate of .55 lb/lb coal, effectively increasing the oxidizer/coal ratio by 20 percent. Thus the agreement between the two investigations is good. Perry et al. (1950) and Elliott et al. (1952) 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. 24) and in the results of two studies reviewed by Lenzer (1977).

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.

4. Post-Test Inspection

The cyclone reactor was disassembled and inspected following the completion of series four. The sampling system was in excellent condition; the ceramic fiber and paper filters (Fig. 16) were dirty but intact. The walls of the reaction chamber were coated with an uneven layer of slag about 1/4 inch thick. The slag port was, of course, bridged over.

Sometime after the start of series four the exhaust throat tube (Fig. 12) broke loose from the top piece of refractory and fell into the reaction chamber; the exhaust gases then left the reactor through a narrow gap which opened up between the top two refractory sections (Fig. 12). The time during the test at which this took place cannot be determined since no change in reactor behavior was observed. The effect of this change in configuration was to force the gases to leave the reactor not along the centerline but through the outer wall where they would be much more likely to carry unreacted particles out with them. Under most conditions, the effect on reactor performance would more than likely be detrimental; however, under the strongly fuel-rich conditions of this test, the carbon efficiency is mainly determined by oxygen depletion and the exhaust composition by water-gas equilibrium. Since the oxygen level in the product gas was negligible (Table 22) and the product gas was very close to water-gas equilibrium (Fig. 27) the effect on reactor performance was apparently minimal.

CHAPTER VI. CONCLUSIONS AND RECOMMENDATIONS

This report describes a unified experimental/analytical investigation of pulverized coal combustion and gasification in a cyclone reactor. The work is unique in that no other investigators have reported a detailed comparison between experiment and theory for a cyclone reactor.

The emphasis in the experimental portion of the program was directed toward coal combustion and gasification via fuel-rich combustion with air at atmospheric pressure. Carbon efficiencies during coal combustion tests were excellent (90-95%) and were largely insensitive to changes in air flowrate and air/fuel ratio. Under gasification conditions, the carbon efficiency was satisfactory (75-90%) and a readily burnable gas was produced.

No peak was observed in the product gas heating value over the range of stoichiometries investigated. The heating value corresponding to the optimum hot and cold gas efficiencies (75 and 45 percent, respectively) was approximately 70 BTU/scf, only 20 percent less than the maximum value observed. The corresponding carbon efficiency was 83 percent, also quite satisfactory.

Slag accumulation in the bottom of the reactor and in the throat tube 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. Solutions to the slag problem that should be investigated in the future include bleeding a small portion of the combustion gases out through the slag port or using a small methane torch to keep the port clear. Reducing the slag viscosity by adding limestone to the incoming coal is also a possible solution: this method offers the dual benefit of simultaneously reducing the levels of SO_2 and NO_x in the product gas (Vogel et al., 1974). Undue time should not be spent on this problem; successful slagging has been amply

demonstrated on a slightly larger scale, and the more important goals of this study can still be achieved without successful slagging.

Future experiments should be directed toward coal gasification (a) via fuel-rich combustion and (b) with moderate steam addition. High air flowrates are desirable to improve carbon efficiency through greater centrifugal effects and to reduce gas residence time so that the product gas heating value can be enhanced by kinetic effects. Experiments could proceed toward lower air/fuel ratios to determine if there is a maximum achievable make gas heating value. Higher heating values must not be obtained, however, at the cost of significantly reducing the carbon, cold and hot gas efficiencies. Internal probing should be used to facilitate more detailed comparisons with the model results. Gasification with steam and oxygen should be considered as a long-term objective.

Modeling efforts were directed toward improving and expanding the cyclone coal combustion model of Thomas (1978). The model now includes a realistic coal pyrolysis treatment and is capable of modeling coal gasification via fuel-rich combustion. The addition of a gas-phase equilibrium model makes it possible to check the kinetic results of the model against the limitations imposed by equilibrium; the equilibrium model is also a vital component in the treatment of the very fuel-rich cases. The agreement between theoretical and experimental results is very good for both combustion and gasification. The agreement under gasification conditions implies that gas phase equilibrium is a good approximation at the moderate residence times of this investigation.

Future efforts with the model should be directed toward predicting the effects of changes in reactor configuration and operating technique; the model should become a tool for selecting the optimum combination of the various system parameters. Already several important conclusions can be reached based on the investigations to date: (1) high air flowrates enhance carbon efficiency by increasing the amount of carbon burned in the PSR zone and are thus beneficial for both combustion and gasification conditions; (2) high air flowrates could also improve gasification results by keeping the reactions from reaching equilibrium; (3) for coal combustion, a significant length of uncooled exhaust line

(a long PFR zone) should be provided to improve carbon efficiency via rapid high-temperature char kinetics and (4) an obvious tradeoff exists between high make gas heating value and high carbon efficiency, cold gas efficiency and hot gas efficiency; the optimum operating point based on the work to date appears to be at roughly 50 percent of stoichiometric air.

There seems little to be gained by increasing the sophistication of the cyclone fluid mechanics model since the present model works so well. However, further experimental results may point out weaknesses in the fluid mechanics treatment, especially at higher flowrates. The addition of steam and CO_2 char kinetics to improve the modeling of very fuel-rich cases is the first step that should be taken in revising the model.

The model as it now stands can be applied to virtually any slagging, vortex coal reactor, with only minor changes in the reactor configuration. Many proposed gasification systems use a cyclone or similar reactor to combust or gasify char or coal: the Combustion Engineering and BIGAS processes, for example, both use slagging cyclones as the first stage of two-stage gasification processes (National Academy of Sciences, 1977).

The future of cyclone reactors in coal conversion processes is bright. Large commercial applications include coal combustion in MHD cycles (Way, 1974) and gasification as part of a combined cycle power plant (National Academy of Sciences, 1977). Perhaps even more important are intermediate and small scale industrial applications to which cyclones are ideally suited. Getschow (1979) reports that some industries are already building "backyard" coal gasifiers for process heat and steam raising as a hedge against future oil and natural gas curtailments. The unique load flexibility of small industrial installations is cited as a primary advantage over large, centralized facilities. Cyclones, with great stability over wide ranges of flowrates and the ability to burn or gasify not only coal but a host of alternate fuels as well, are well-suited toward fulfilling a much needed role in the future use of solid fossil fuels.

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APPENDIX A: MODEL CALCULATION PROCEDURE AND PROGRAM LISTING

The calculation procedure used for the cyclone model is outlined in this appendix.. Comment cards are used extensively throughout the program to assist in examination or use. The program is written in such a way that the user can dictate the level of complexity of the model by choosing various options within the program. Those steps which can be bypassed by the user are indicated with an asterisk in the following procedure outline.

The program consists of a main program and seven major subroutines, some of which utilize other subprograms and Purdue University computer library routines. Table 11 provides a brief description of the main program and the major subroutines.

A. Calculation Procedure

1. Initialize values for air and coal input flowrates and temperatures, coal composition, particle size distribution and cyclone geometry.
2. Choose appropriate program options and establish an initial value for the flame temperature T_f .

Pyrolysis Zone

3. Perform a pyrolysis analysis based on the constant volatiles mass fraction model (subroutine PYRO). Calculate char and gaseous species flowrates and heat released via volatiles combustion.

*4. Perform a detailed pyrolysis analysis using the Kobayashi weight loss model. The pyrolysis zone gas temperature is assumed equal to the current value of the flame temperature. Calculate char and gaseous species flowrates and heat released via volatiles combustion.

Table 11. Computer Model Main Program and Subroutines

<u>Name</u>	<u>Function</u>
MAIN	Reads input data and flags for choosing options. Performs heat transfer analysis.
PYRO	Calculates volatiles yield and char and gaseous species flowrates based on the assumption of a constant volatiles mass fraction.
PYR02	Uses the pyrolysis model of Kobayashi et al. (1977) and a particle heating model to calculate a realistic volatiles yield.
TEMP	Calculates gas temperatures via an energy balance using integrated heat capacity equations.
PSR	Calculates gas composition, char flowrate and temperature for the PSR zone.
PFR	Calculates gas composition, char flowrate and temperature throughout the PFR zone.
EQLDRM	Calculates equilibrium gas-phase composition and temperature and compares to kinetic values.
GASPAR	Calculates heating value, cold and hot gas efficiency and make gas yield for fuel-rich runs.

PSR Zone

5. The convective plus radiative heat transfer from the pressure vessel is found. An initial guess for the vessel temperature T_o is used to begin the calculations.

6. Using the heat transfer value of step 5 and the current value of the flame temperature T_f , the inner reactor wall temperature T_w is found.

7. Using T_w from step 6, the conductive heat transfer through the walls is calculated.

8. The heat transfer through the port openings is calculated.

9. Heat transfer from the pressure vessel (step 5) is compared to heat transfer through the walls for the assumed T_f . A new value for T_o is chosen. Calculations return to step 5 until a consistent set of heat transfer parameters is found.

10. The total heat loss rate out of the PSR zone is found.

11. The size of particles leaving the PSR zone is calculated, assuming enough oxygen is present to convert all the carbon released to CO.

12. The amount of carbon released via the force balance treatment is calculated and compared to the amount of oxygen available.

13. If the oxygen supply is inadequate for conversion to CO, the amount of carbon released is reduced accordingly. The chemical heat release rate is found. Gas-phase composition and temperature are determined by an equilibrium analysis. Gasification parameters are calculated, and the analysis skips to step 18.

14. If the oxygen supply is sufficient, mass balances for CO, O_2 and CO_2 for the PSR zone are performed.

a. Gas concentrations are calculated.

b. The rate of CO combustion is found.

c. Flowrates of CO, CO_2 and O_2 out of the PSR zone are calculated.

15. The chemical heat release rate is found.

*16. The PSR zone (flame) temperature is calculated.

*17. The PSR zone results are compared with the results of an equilibrium analysis based on the same T_f . The kinetic results are used in

succeeding calculations only if they are not in violation of the second law, in which case the equilibrium results are used. The equilibrium results are also used if the oxygen supply is depleted.

*18. The flame temperature of step 17 (or step 13) is compared to the previous value of the flame temperature. If the values are within a certain tolerance, calculations proceed to step 19; otherwise, they return to step 4. The iteration process continues until convergence is achieved.

PFR Zone

19. The flow of each constituent into either the first or next volume increment of the PFR zone is calculated.

20. Mass balances are performed for a particular volume increment of the PFR zone.

- a. Gas concentrations of H_2O , CO and CO_2 are found.
- b. Char and CO combustion rates are calculated.
- c. Flows of CO, CO_2 , O_2 and char out of the volume increment are calculated.

*21. The chemical heat release rate and temperature for the volume increment are found.

*22. The results for the volume increment are compared with the results of an equilibrium analysis. The kinetic results are used in succeeding calculations only if they are not in violation of the second law, in which case the equilibrium results are used. The equilibrium results are also used if the oxygen supply is depleted.

23. Steps 19 through 22 are repeated for each succeeding volume increment to the end of the PFR zone.

B. Program Listing

	EXTERNAL FCN	A	10
	REAL KGAS,NI,MOL02,MOLN2,MOLUC,MOLCC,MOLN,MOLH,MOLS,MOLO,NO,MOUJT,	A	20
	IN2,MCO,MCO2,M02,KP1,KP2,MOLWTR	A	30
	COMMON /A/ IFLAG	A	40
	COMMON /B/ DCAR,S,EXPAN,FLOCOL,FUOL,CYCL,CYCR,TROR,TROL,EXAIR,RCRT	A	50
	COMMON /C/ FLOPRI,FLOSEC,TPRI,TSEC,ASH	A	60
	COMMON /D/ KFLAG	A	70
	COMMON /E/ GASIND	A	80
	COMMON /H/ EXAIR2,FLOCL2	A	90
	COMMON /UNITS/ NUNITS	A	100
	DIMENSION X0(5), ALPHA(5)	A	110
	NUNITS=7	A	120
101	CONTINUE	A	130
	READ (5,111) CARB,HY,NI,SU,ASH,OX,WATER,CHU	A	140
	IF (CARB.LT..1) GO TO 110	A	150
	READ (5,114) DCAR,S,FBF	A	160
C		A	170
C	READ COAL COMPOSITION IN WT PERCENT C, H, N, S, ASH, O, WATER.	A	180
C	READ COAL HEATING VALUE IN BTU/LB.	A	190
C	THE LAST DATA CARD MUST BE A BLANK	A	200
C	CARD TO SIGNAL THE COMPUTER TO STOP.	A	210
C	READ IN POSIN RAMMLER DIST PARAMETERS AND FORCE BALANCE FACTOR	A	220
C	UNITS OF DCAR ARE MICRONS.	A	230
C	READ MASS FLOW (LB/HR) INPUT FOR PRIMARY AIR, SECONDARY AIR AND	A	240
C	COAL, AND THEIR RESPECTIVE TEMPERATURES IN DEGREES R.	A	250
C	READ VOLATILES FRACTION AND COAL EXPANSION COEFFICIENT	A	260
C		A	270
	READ (5,115) FLOPRI,FLOSEC,FLOCOL,TPRI,TSEC	A	280
	FLOCL2=FLOCOL	A	290
	READ (5,112) FUOL,EXPAN	A	300
	READ (5,113) CYCL,CYCR,TROL,TROR,ANOZ	A	310
C		A	320
C	READ CYCLONE LENGTH AND RADIUS, THROAT LENGTH AND RADIUS, AND	A	330
C	TOTAL NOZZLE AREA, IN FT AND FT2.	A	340
C	READ WALL, FLAME AND VESSEL EMISSIVITIES, INITIAL VESSEL TEMPERATU	A	350
C	GUESS, AMBIENT TEMPERATURE AND FLAME TEMPERATURE	A	360
C		A	370
	READ (5,111) EM,EF,FU,TUI,TAMB,TF	A	380
	TSAJE=TF	A	390
C		A	400
C	IFLAG = 1 FOR ISOTHERMAL CASE, 0 FOR NONISOTHERMAL CASE	A	410
C	IF KFLAG = 1, EQUILIBRIUM EFFECTS ARE CONSIDERED.	A	420
C	IF KFLAG = 0 THEY ARE NOT.	A	430
C	IF IPYR EQUALS ONE THE FINAL PYROLYSIS SUBROUTINE IS USED.	A	440
C	IF IPYR EQUALS ZERO IT IS NOT.	A	450
C	AW - REACTOR WALL AREA, FT2, QIN - VOLUME FLOW OF AIR IN FT3/HR,	A	460
C	UIN - AIR INLET VELOCITY, FT/S	A	470
C		A	480
	READ (5,116) IFLAG,KFLAG,IPYR	A	490
	J=0	A	500
	JKL=0	A	510
	TU=TUI	A	520
	PI=3.14159	A	530
	AW=2.*PI*CYCR*(CYCR+CYCL)	A	540
	QIN=(FLOPRI*TPRI+FLOSEC*TSEC)*0.02517/3600.	A	550
	RU=PI*CYCL*CYCR**2	A	560
	UIN=QIN/ANOZ	A	570
	NFLAG=2	A	580
	WRITE (6,117)	A	590
	WRITE (6,133) IFLAG,KFLAG	A	600

	IF (IFLAG.EQ.0) WRITE (6,134)	A 610
	IF (IFLAG.EQ.1) WRITE (6,135)	A 620
	IF (KFLAG.EQ.0) WRITE (6,136)	A 630
	IF (KFLAG.EQ.1) WRITE (6,137)	A 640
	IF (IPYR.EQ.0) WRITE (6,138)	A 650
	IF (IPYR.EQ.1) WRITE (6,139)	A 660
	WRITE (6,118) CYCL,CYCR,TROL,TROR	A 670
	WRITE (6,119) EU,EF,EU,TUI,TAMB,TF	A 680
	WRITE (6,120) CARB,HY,NI,SU,OX,ASH,WATER	A 690
	WRITE (6,121) FLOPRI,FLOSEC,FLOCOL,TPRI,TSEC	A 700
	FLOAIR=(FLOPRI*FLOSEC)/29.	A 710
	MOLO2=FLOAIR*0.21	A 720
	MOLN2=FLOAIR*0.79	A 730
	WRITE (6,122) FLOAIR,MOLC2,MOLN2	A 740
	EXAIR=MOLO2*100./((FLOCOL*(CARB/12.+SU/32.+5*NI/14.+25*HY-.5*OX/16.))	A 750
	16.))	A 760
C		A 770
C	EXAIR = AIR/FUEL DIVIDED BY STOICHIOMETRIC AIR/FUEL.	A 780
C		A 790
	EXAIR2=EXAIR	A 800
	WRITE (6,123) EXAIR	A 810
C		A 820
C	PERFORM PRELIMINARY PYROLYSIS ANALYSIS.	A 830
C		A 840
	CALL PYRO (MOLO2,MOLN2,CO,H2O,NO,SO2,OX2,HEAT,TOUT1,HTOT1,FLOCOL,F	A 850
	1UOL,CHU,FRAC,CARB,HY,NI,SU,OX,WATER)	A 860
	WRITE (6,124) H2O,CO,NO,SO2,OX2,MOLN2,HEAT	A 870
	WRITE (6,125) TOUT1	A 880
	TFLOW=OX2+CO+H2O+NO+SO2+MOLN2	A 890
	DENSAS=1./((72*TF)	A 900
	VOLFLO=TFLOW/DENSAS	A 910
	VOLPYR=PI*.167*(CYCR**2-TROR**2)	A 920
	RTPYR=VOLPYR*3600./VOLFLO	A 930
C		A 940
C	TOTAL GAS FLOW, LBMOLE/HR.	A 950
C	GAS DENSITY, LBMOLE/FT**3.	A 960
C	VOLUMETRIC FLOWRATE, FT**3/HR.	A 970
C	PYROLYSIS ZONE VOLUME, FT**3.	A 980
C	PYROLYSIS ZONE RESIDENCE TIME, SEC.	A 990
C	BEGIN OUTERMOST LOOP FOR FLAME TEMPERATURE CONVERGENCE	A 1000
C	PERFORM MORE SOPHISTICATED PYROLYSIS ANALYSIS.	A 1010
C		A 1020
	102 CONTINUE	A 1030
	IF (IPYR.EQ.1) CALL PYRO2 (RTPYR,CARB,HY,NI,SU,OX,WATER,CHU,NO,SO2	A 1040
	1,OX2,CO,H2O,HTOT1,MOLO2,MOLN2,TF,FRAC)	A 1050
	FLAG=0.0	A 1060
	TH=TF-30.	A 1070
	G=(FLOPRI*FLOSEC)*TF*0.02517/2600.	A 1080
	UEFF=G/ANDZ	A 1090
	RT=RV/G	A 1100
C		A 1110
C	QOUT - VOLUME FLOW OF AIR AT FLAME TEMP., FT3/S, UEFF - EFFECTIVE	A 1120
C	NOZZLE VELOCITY, FT/S, RT - GAS RESIDENCE TIME.,S	A 1130
C	CALCULATE HEAT TRANSFER OFF PRESS. VESSEL	A 1140
C		A 1150
	WRITE (6,126)	A 1160
	THEAN=(TU+TAMB)/2.	A 1170
103	DYUISC=.000233+.000139*(THEAN-660.)/200.	A 1180
	TDELT=TU-TAMB	A 1190
C		A 1200

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C      COEFFICIENT = PR*CL**3                      A 1210
C                                                    A 1220
C      GRPRH=860.1*TDEL/(TMEAN*DYUISC**2)          A 1230
C      GRPRV=950.4*TDEL/(TMEAN*DYUISC**2)          A 1240
C      A=EU*.1714*25.92/100000000.                A 1250
C      HU=.19*(TDEL**3333)                          A 1260
C      HNU=.27*((TDEL/2.650)**.25)                  A 1270
C      HHL=.12*((TDEL/1.772)**.25)                  A 1280
C                                                    A 1290
C      TEST FOR LAMINAR OR TURBULENT FREE CONVECTION A 1300
C                                                    A 1310
C      IF (GRPRH.GT.1000000000.) HNU=.22*(TDEL**3333) A 1320
C      IF (GRPRV.LT.1000000000.) HU=.29*((TDEL/2.75)**.25) A 1330
C      B=HU*17.23+HNU*7.07+HHL*3.14                A 1340
C      QAFREE=B*TDEL                                 A 1350
C      QARAD=A*(TU**4-TAMB**4)                      A 1360
C      QTOT1=QAFREE+QARAD                           A 1370
C      C=A*TAMB**4+B*TAMB                           A 1380
C                                                    A 1390
C      TMEAN - AVERAGE BOUNDARY LAYER TEMPERATURE, DYUISC - DYNAMIC A 1400
C      VISCOSITY OF AIR, FT**2/S (KREITH), GRPRH, GRPRV - GRASHOF*PRANDTL A 1410
C      NUMBERS FOR HORIZONTAL AND VERTICAL SURFACES, HU, HNU, HHL - FREE A 1420
C      CONVECTION COEFFICIENTS FOR A HEATED VERTICAL PLATE, HORIZONTAL A 1430
C      PLATE FACING UPWARD, AND HORIZONTAL PLATE FACING DOWNWARD A 1440
C      RESPECTIVELY, BTU/HR*FT**2, QAFREE, QARAD - FREE CONVECTION AND A 1450
C      RADIATION HEAT TRANSFER OFF THE PRESSURE VESSEL, BTU/HR, QTOT1 - A 1460
C      TOTAL HEAT TRANSFER OFF THE PRESSURE VESSEL, BTU/HR. A 1470
C      REACTOR WALL HEAT TRANSFER A 1480
C                                                    A 1490
C      TAVE=(TF+TW)/2.                               A 1500
C      DYUISC=.00214+.00125*(TAVE-2460.)/1000.      A 1510
C      KGAS=.047+.007*(TAVE-2460.)/1000.           A 1520
C      RE=UEFF*PI*2.*CYCR/DYUISC                    A 1530
C      HWALL=.036*RE**0.8*0.914*KGAS/1.571          A 1540
C      EEFF=1./((1./EF)*(1./EW)-1.)                 A 1550
C      D=AW*.1714*EEFF/100000000.                  A 1560
C      E=HWALL*AW                                     A 1570
C      F=D*TF**4+E*TF                                A 1580
C                                                    A 1590
C      EF - FLAME EMISS, DYUISC - DYNAMIC VISCOSITY OF AIR, FT2/S (KREITH) A 1600
C      KGAS - AIR THERMAL CONDUCTIVITY, BTU/HR-FT-R, RE - RENOLDS NUMBER, A 1610
C      HWALL - FORCED CONVECTION H T COEFFICIENT, BTU/HR-FT2-R, EEFF - A 1620
C      EFFECTIVE FLAME EMISSIVITY. A 1630
C      CALC WALL TEMP FROM FLAME TEMP AND QTOT1 A 1640
C                                                    A 1650
C      NJ=0 A 1660
C      104 TWNEW=((F-QTOT1-E*TW)/D)**.25 A 1670
C      IF (ABS(TW-TWNEW).LT..1) GO TO 105 H 1680
C                                                    A 1690
C      CHECK FOR TEMPERATURE CONVERGENCE A 1700
C                                                    A 1710
C      TW=(TW+TWNEW)/2. A 1720
C      NJ=NJ+1 A 1730
C      GO TO 104 A 1740
C      105 CONTINUE A 1750
C                                                    A 1760
C      CALC HEAT TRANSFER TO THE REACTOR WALLS A 1770
C                                                    A 1780
C      QACONV=E*(TF-TW) A 1790
C      QAF=D*(TF**4-TW**4) A 1800

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C		A 1810
C	QACONV, QAF - CONDUCTIVE AND RADIATIVE HEAT TRANSFER TO THE REACTO	A 1820
C	WALL, BTU/HR.	A 1830
C	CALC CONDUCTIVE HEAT TRANSFER	A 1840
C		A 1850
	QTOT2=(TM-TU)*.725/.278	A 1860
	FLAG=FLAG+1.	A 1870
	QTOT3=.0222*.1714*EF*(TF**4-1000.**4)/100000000.	A 1880
C		A 1890
C	QTOT2 - CONDUCTIVE TRANSFER THROUGH THE REACTOR, BTU/HR.	A 1900
C	QTOT3 - RADIATIVE HEAT LOSS THROUGH THE SLAG TAP AND THROAT, BTU/H	A 1910
C	CHECK IF HEAT TRANSFER IS CONSISTENT	A 1920
C		A 1930
	IF (ABS(QTOT2/QTOT1-1.00).LT..002) GO TO 107	A 1940
	IF (FLAG.GT.25.) GO TO 107	A 1950
	QTOTAU=(QTOT1+QTOT2)/2.	A 1960
	I=0	A 1970
C		A 1980
C	CALC NEW TU FROM QTOTAU	A 1990
C		A 2000
	106 TUNEW=((QTOTAU+C-E*TU)/A)**.25	A 2010
	IF (ABS(TU-TUNEW).LT.0.1) GO TO 103	A 2020
	TU=(TU+TUNEW)/2.	A 2030
	T=T+1	A 2040
	GO TO 106	A 2050
	107 CONTINUE	A 2060
	QTOT=QTOTAU+QTOT3	A 2070
C		A 2080
C	QTOT - TOTAL HEAT LOSS, BTU/HR	A 2090
C	CALC CRITICAL PARTICLE DIAMETER	A 2100
C		A 2110
	WRITE (6,127) QTOT	A 2120
	UISC=(3.45+0.41*(TF-2460.)/1000.)/100000.	A 2130
	DENCOL=85.0*(1.-FUDL)/EXPA**3	A 2140
	AA=3.0*(CYCL-TRCL)*(CYCR-TRCR)*TRCR/CYCR	A 2150
	BB=SQRT(UISC/(Q*PI*CYCL*DENCOL))	A 2160
	DCRIT=AA*BB*FDF	A 2170
	DCRITM=DCRIT*304300.	A 2180
C		A 2190
C	UISC - AIR VISCOSITY, LBM/FT-S (KREITH), DENCOL - COAL DENSITY AFT	A 2200
C	SWELLING AND PYROLYSIS, LB/FT3. DCRIT, DCRITM - CRITICAL PARTICLE	A 2210
C	DIAMETER IN FT AND MICRONS RESPECTIVELY.	A 2220
C		A 2230
	RCRT=TROR	A 2240
	WRITE (6,128) DCRITM	A 2250
	CALL PSR (DCRITM,BURNT,BURN,MOUTT,CO,H2O,NO,SO2,OX2,MOLN2,HTOT1,FR	A 2260
	1AC,TF,QTOT,TFNEW,MCO,MCO2,MO2,HTOT2,CHU,XO,ALPHA,H2)	A 2270
	WRITE (6,129) BURN,BURNT,MOUTT	A 2280
	WRITE (6,130) RT	A 2290
C		A 2300
C	CHECK FOR FLAME TEMPERATURE CONVERGENCE	A 2310
C		A 2320
	IF (ABS(TFNEW-TF).LT.5.) GO TO 109	A 2330
	TSAVE2=TSAVE	A 2340
	TSAVE=TF	A 2350
	IF (ABS(TFNEW-TSAVE2).LT.5.) TF=.5*(TF+TFNEW)	A 2360
	IF (ABS(TFNEW-TSAVE2).GE.5.) TF=TFNEW	A 2370
	J=J+1	A 2380
	IF (J.GT.20) GO TO 108	A 2390
	GO TO 102	A 2400

108	CONTINUE	A	2410
	JKL=JKL+1	A	2420
	IF (JKL.EQ.1) TF=TF+500.	A	2430
	IF (JKL.EQ.2) TF=TF-500.	A	2440
	IF (JKL.EQ.3) WRITE (6,131)	A	2450
	IF (JKL.EQ.3) GO TO 110	A	2460
	J=0	A	2470
	GO TO 102	A	2480
109	WRITE (6,132) TFNEW	A	2490
	IF (GASIND.GT.0.) GO TO 101	A	2500
	N2=MOLN2	A	2510
	CALL PFR (DCRITH,RCRT,CYCL,TROR,DENCOL,FRAC,H2O,MCO,N2,MO2,MCO2,NO	A	2520
	1,SO2,TFNEW,MOUTT,HTOT2,TROL,CHU,X0,ALPHA,H2)	A	2530
	GO TO 101	A	2540
110	STOP	A	2550
C		A	2560
111	FORMAT (2F10.0)	A	2570
112	FORMAT (2F10.0)	A	2580
113	FORMAT (5F10.0)	A	2590
114	FORMAT (3F10.0)	A	2600
115	FORMAT (5F10.0)	A	2610
116	FORMAT (3I3)	A	2620
117	FORMAT (1H1,10X, 22H*** INITIAL CALCULATIONS ***)	A	2630
118	FORMAT (1X,18HCYCLONE DIMENSIONS,4(5X,F10.6))	A	2640
119	FORMAT (5X,3HEM=,F6.3,5X,3HEF=,F6.3,5X,2HEU,F6.3,5X,4HTUI=,F6.1,5X	A	2650
	1,5HTAMB=,F6.1,5X,3HTF=,F6.1)	A	2660
120	FORMAT (1X,16HCOAL COMPOSITION,5X,2HC=,F6.3,5X,2HH=,F6.3,5X,2HN=,F	A	2670
	16.3,5X,2HS=,F6.3,5X,2HO=,F6.3,5X,3HASH,F6.3,5X,6HWATER=,F6.3)	A	2680
121	FORMAT (1X,20HMASS FLOWRATES LB/HR,5X,5HPRIM=,F6.2,5X,4HSEC=,F7.2,	A	2690
	15X,5HCOAL=,F10.5,10X,6HTPRIM=,F6.1,5X,5HTSEC=,F6.1)	A	2700
122	FORMAT (1X, 32HAIR, OXYGEN, AND NITROGEN MOLAR , 22HFLOWRATES IN L	A	2710
	1BMOL/HR,2X,3F12.4)	A	2720
123	FORMAT (1X, 39H(AIR/FUEL)/(STOICHIOMETRIC AIR/FUEL) = ,F6.3)	A	2730
124	FORMAT (1X,8HGAS COMP,3X,4HH2O=,F7.4,3X,3HCO=,F7.4,3X,3HNO=,F7.4,3	A	2740
	1X,4HSO2=,F7.4,3X,3HO2=,F7.4,3X,3HN2=,F7.4,5X,13HHEAT RELEASE=,F12.	A	2750
	22)	A	2760
125	FORMAT (1X,21HTEMP AFTER PYROLYSIS=,F10.2,/))	A	2770
126	FORMAT (/,10X,35H *** HEAT TRANSFER CALCULATIONS ***,/)	A	2780
127	FORMAT (/,1X,23HTOTAL HEAT LOSS, BTU/HR,3X,F12.3)	A	2790
128	FORMAT (/,15X,28HCRITICAL DIAMETER (MICRONS)=,F10.5)	A	2800
129	FORMAT (1X,24HTOTAL MASS BURNT IN PSR=,F10.6,10X,18HTOTAL MASS BU	A	2810
	1RNT=,F10.6,10X,15HTOTAL MASS OUT=,F10.6)	A	2820
130	FORMAT (1X,18HGAS RESIDENCE TIME,E15.8)	A	2830
131	FORMAT (5X,22HNO OVERALL CONVERGENCE)	A	2840
132	FORMAT (/,5X,20HCONVERGENCE COMPLETE,5X,15HFINAL PSR TEMP=,F8.1)	A	2850
133	FORMAT (/,10X, 8HIFLAG = ,I2, 10H KFLAG = ,I2,/))	A	2860
134	FORMAT (10X, 13HNONISOTHERMAL)	A	2870
135	FORMAT (10X, 10HISOTHERMAL)	A	2880
136	FORMAT (10X, 34HEQUILIBRIUM EFFECTS NOT CONSIDERED)	A	2890
137	FORMAT (10X, 30HEQUILIBRIUM EFFECTS CONSIDERED)	A	2900
138	FORMAT (10X, 34HFINAL PYROLYSIS MODEL NOT INCLUDED)	A	2910
139	FORMAT (10X, 30HFINAL PYROLYSIS MODEL INCLUDED)	A	2920
C		A	2930
	END	A	2940
	SUBROUTINE PYRO (O2,N2,CO,H2O,NO,SO2,OX2,HEAT,TOUT,HTOT,COAL,FU,CH	B	10
	1U,FRAC,CARB,HY,NI,SU,OX,WATER)	B	20
	REAL NO,N2,MASS,MOLUC,MOLCC,MOLN,MOLH,MOLS,MOLU,MOLWTR,NI	B	30
	COMMON /C/ PRI,SEC,TP,TS,ASH	B	40
	WRITE (6,101)	B	50
	UCARB=FU*(CARB+ASH)+(FU-1.)*(HY+NI+SU+OX+WATER)	B	60

	CHARC=CARB-UCARB	B	70
	FRAC=CHARC/(100.-HY-NI-SU-OX-UCARB-WATER)	B	80
C		B	90
C	CALCULATE VOLATILE COMPOSITION	B	100
C	UCARB, CHARC - WT PERCENT CARBON IN VOLATILES AND CHAR RESPECTIVELY	B	110
C	FRAC - FRACTION OF CHAR WHICH IS CARBON.	B	120
C	CALC MOLAR FLOWRATES IN LB-MOLES/HR	B	130
		B	140
	MOLUC=UCARB*COAL/1200.	B	150
	MOLCC=CHARC*COAL/1200.	B	160
	MOLN=NI*COAL/1400.	B	170
	MOLH=HY*COAL/100.	B	180
	MOLS=SU*COAL/3200.	B	190
	MOLO=OX*COAL/1600.	B	200
	MOLWTR=WATER*COAL/1800.	B	210
C		B	220
C	CALCULATE MOLAR FLOW OF GASES AFTER PYROLYSIS AND COMBUSTION OF	B	230
C	VOLATILES, LB-MOLES/HR	B	240
C		B	250
	H2=0.	B	260
	CO2=0.0	B	270
	NO=MOLN	B	280
	CO=MOLUC	B	290
	H2O=MOLH/2.+MOLWTR	B	300
	SO2=MOLS	B	310
	OX2=O2-.5*(CO+MOLH/2.+NO-MOLO)-SO2	B	320
C		B	330
C	CALCULATE HEAT RELEASE IN BTU/HR	B	340
C		B	350
	HEAT=COAL*(CHU-(1.-FU)*FRAC*14110.)-CO*121750.	B	360
	TR=500.	B	370
C		B	380
C	CALC INPUT ENTHALPY	B	390
C	INTEGRATED SPECIFIC HEAT EQUATIONS (WARK P68).	B	400
C		B	410
	DHP=6.557*(TP-TR)+.0004103*(TP**2-TR**2)-2.21E-8*(TP**3-TR**3)	B	420
	DHS=6.557*(TS-TR)+.0004103*(TS**2-TR**2)-2.21E-8*(TS**3-TR**3)	B	430
	DHC=0.30*(TP-TR)	B	440
	FLODH=DHP*PRI/29.+DHS*SEC/29.+DHC*COAL	B	450
C		B	460
C	TR - REFERENCE TEMP., DEG R, DHP, DHS, DHC - INPUT ENTHALPY OF	B	470
C	PRIMARY AIR, SECONDARY AIR AND COAL, BTU/LB. FLODH - INPUT ENTHAL	B	480
C	BTU/HR	B	490
C	HTOT - TOTAL ENTHALPY OF GAS RELATIVE TO TR, BTU/HR.	B	500
C	CASH - CHAR + ASH FLOW, LB/HR.	B	510
C		B	520
	HTOT=HEAT+FLODH	B	530
	CASH=COAL*(1.-FU+FU*ASH/100.)	B	540
	CALL TEMP (CO,CO2,H2,H2O,NO,N2,O2,SO2,CASH,HTOT,TR,1000.,T)	B	550
	TOUT=T	B	560
	WRITE (6,102) CO,CO2,H2,H2O,NO,N2,OX2,SO2,CASH,FRAC,FU,HEAT	B	570
	RETURN	B	580
C		B	590
	101 FORMAT (////,10X, 42H*** PRELIMINARY PYROLYSIS CALCULATIONS ***,/)	B	600
	102 FORMAT (1X, 26HGAS FLOWRATES, LBMOL/HR, , 41HAFTER PYROLYSIS AND	B	610
	1VOLATILES COMBUSTION-,,1X, 38HCO, CO2, H2, H2O, NO, N2, O2, AND S	B	620
	2O2.,,,10X,8E12.3,,,1X, 22HCHAR FLOWRATE, LB/HR, , 30HAND CHAR CAR	B	630
	3BON MASS FRACTION.,,,10X,2E12.3,,,1X, 24HVOLATILES MASS FRACTION	B	640
	4, 40HAND HEAT RELEASE VIA VOLATILES BURNING, , 7HBTU/HR.,,,10X,2E	B	650
	512.3,///)	B	660

C	END	B	670
	SUBROUTINE PYR02 (RTPYR,CARB,HY,NI,SU,OX,WATER,CHU,NO,SO2,OX2,CO,H	B	680
	120,HTPYR2,MOL02,MOLN2,TF,FRAC)	C	10
	REAL NI,MOLCC,MOLUC,MOLH,MOLH,MOL0,MOLS,MOLWTR,NO,MOL02,MOLN2,KGAS	C	20
	REAL K1B,K2B,K1E,K2E	C	30
	COMMON /B/ DCAR,S,EXPAN,FLOCOL,FUOL,CYCL,CYCR,TROF,TROL,EXAIR,RCRT	C	40
	COMMON /C/ FLOPRI,FLOSEC,TPRI,TSEC,ASH	C	50
	WRITE (6,105)	C	60
C		C	70
C	INLET CONDITIONS ARE AS FOLLOW. PRIMARY AND SECONDARY AIR FLOW,	C	80
C	FLOPRI, FLOSEC, IN LB/HR, AT TEMPERATURES TPRI, TSEC. COAL FLOW I	C	90
C	LB/HR, FLOCOL, AT TEMPERATURE TPRI. COAL MASS FRACTION PERCENTAGE	C	100
C	CARB, HY, NI, SU, OX, WATER, ASH, AND HEATING VALUE CHU IN BTU/LB	C	110
C	AS RECEIVED. APPROXIMATE PYROLYSIS ZONE GAS RESIDENCE TIME, RTPYR	C	120
C	SEC. TOTAL AIR FLOW, FLOAIR, IN LBMOL/HR, N2 AND O2 FLOWS,	C	130
C	MOLN2 AND MOL02, LBMOL/HR.	C	140
C		C	150
	KPYR=0	C	160
	PARTRT=10.*RTPYR	C	170
C		C	180
C	PARTICLE RESIDENCE TIME IS ARBITRARILY ASSUMED TO BE	C	190
C	TEN TIMES GAS RESIDENCE TIME.	C	200
C	INITIALIZE VARIABLES.	C	210
C		C	220
	DIA=EXPAN*DCAR*(ALOG(2.))**(1./S)/304800.	C	230
	TPYR2=TF	C	240
	PMAS=FLOCOL	C	250
	UMAS=0.	C	260
	PTEMP=TPRI	C	270
	PTIME=0.	C	280
	INT=1	C	290
C		C	300
C	PARTICLE DIAMETER IN FEET.	C	310
C	PYROLYSIS ZONE TEMPERATURE, DEG R.	C	320
C	PARTICLE AND VOLATILES MASSES, LB/HR, AND PARTICLE TEMPERATURE, R.	C	330
C	ACCUMULATED PYROLYSIS TIME, SEC.	C	340
C	INTERVAL COUNTER.	C	350
C		C	360
	ALPHA1=.3*(100.-ASH-WATER)/(100.-ASH)+WATER/(100.-ASH)	C	370
	ALPHA2=(100.-ASH-WATER)/(100.-ASH)	C	380
C		C	390
C	MODIFIED KOBAYASHI VOLATILES MASS FRACTIONS.	C	400
C		C	410
	FUL=0.	C	420
C		C	430
C	FUL IS THE MASS FRACTION VOLATILIZED.	C	440
C		C	450
	101 CONTINUE	C	460
	DENCOL=85.*(1.-FUL)/EXPAN**3	C	470
	TMEAN=(PTEMP+TPYR2)/2.	C	480
	KGAS=(1.774E-5)*TMEAN*.00619	C	490
C		C	500
C	COAL DENSITY AND GAS THERMAL CONDUCTIVITY.	C	510
C	SUBROUTINE RUNPT FINDS THE PARTICLE TEMPERATURE AT THE END OF THE	C	520
C	CURRENT INTERVAL.	C	530
C	SMALLER TIME STEPS ARE TAKEN AT FIRST TO INSURE ACCURACY.	C	540
C		C	550
	IF (INT.LT.61) DT=PARTRT/2000.	C	560
	IF (INT.GE.61) DT=PARTRT/200.	C	570
		C	580

CALL RUNPT (PTMP,PTMP2,DIA,DENCOL,TF,TPYR2,DT,KGAS)	C 580
IF (PTMP2.LT.PTMP) PTMP2=PTMP	C 590
B1=2.E5	C 610
B2=1.3E7	C 620
E1=25.	C 630
E2=40.	C 640
PTB=PTMP*5./9.	C 650
PTE=PTMP2*5./9.	C 660
R=1.986E-3	C 670
K1B=B1*EXP(-E1/(R*PTB))	C 680
K1E=B1*EXP(-E1/(R*PTE))	C 690
K2B=B2*EXP(-E2/(R*PTB))	C 700
K2E=B2*EXP(-E2/(R*PTE))	C 710
	C 720
B VALUES ARE FREEEXPONENTIAL FACTORS.	C 730
E VALUES ARE ACTIVATION ENERGIES.	C 740
K VALUES ARE RATE CONSTANTS.	C 750
	C 760
FWL=((ALPHA1*K1E+ALPHA2*K2E)/(K1E+K2E))*(EXP(-(K1B+K2B)*PTIME)-EXP	C 770
1(-(K1E+K2E)*(PTIME+DT)))	C 780
	C 790
FWL IS THE FRACTIONAL WEIGHT LOSS DURING THE INTERVAL.	C 800
FIND WEIGHT LOSS DURING THE INTERVAL AND ACCUMULATED TOTALS.	C 810
	C 820
WL=FWL*FLOCOL*(1.-ASH/100.)	C 830
UMAS=UMAS+WL	C 840
FUL=UMAS/FLOCOL	C 850
PMAS=FLOCOL-UMAS	C 860
	C 870
FWL IS THE WEIGHT OF VOLATILES EVOLVED PER WEIGHT OF ASH FREE COAL	C 880
DURING THE INTERVAL. WL IS THE WEIGHT LOSS RATE DURING THE INTERU	C 890
UMAS IS THE TOTAL QUANTITY OF VOLATILES EVOLVED, AND PMAS IS THE	C 900
MASS OF CHAR PLUS REMAINING VOLATILES IN LB/HR.	C 910
	C 920
PTIME=PTIME+DT	C 930
PTMP=PTMP2	C 940
INT=INT+1	C 950
IF (PTIME.LE.PARTRT) GO TO 101	C 960
	C 970
PYROLYSIS IS COMPLETED. SEE IF THE MASS AND ENERGY BALANCES	C 980
ARE CONSISTENT.	C 990
	C 1000
IF (FUL.LT.((HY+NI+SU+OX+WATER)/100.)) KPYP=1	C 1010
	C 1020
IF THE FRACTION VOLATILIZED IS LESS THAN THE SUM OF THE HYDROGEN,	C 1030
NITROGEN, SULFUR, OXYGEN, AND MOISTURE MASS FRACTIONS THERE IS	C 1040
TROUBLE.	C 1050
CALCULATE MOLAR FLOWRATES OF VOLATILES AND FIXED CARBON AND THE	C 1060
PRODUCTS OF VOLATILES COMBUSTION. UNITS ARE LBMOL/HR.	C 1070
	C 1080
MOLN=NI*FLOCOL/1400.	C 1090
MOLS=SU*FLOCOL/3200.	C 1100
MOLH=HY*FLOCOL/100.	C 1110
MOLWTR=WATER*FLOCOL/1800.	C 1120
MOLO=OX*FLOCOL/1600.	C 1130
IF (KPYP.EQ.1) GO TO 102	C 1140
CARVOL=UMAS-(NI+SU+HY+OX+WATER)*FLOCOL/100.	C 1150
UCARB=100.*FUL-(HY+NI+SU+OX+WATER)	C 1160
CHARC=CARB-UCARB	C 1170
FRAC=CHARC/(CHARC+ASH)	C 1180

	MOLUC=UCARB*FLOCOL/1200.	C 1190
	MOLCC=CHARC*FLOCOL/1200.	C 1200
C		C 1210
C	THE AMOUNT OF CARBON VOLATILIZED EQUALS THE TOTAL WEIGHT LOSS	C 1220
C	MINUS (NI + HY + SU + OX + WATER).	C 1230
C	CARBOL IS MASS FLOWRATE OF VOLATILIZED CARBON IN LB/HR	C 1240
C	UCARB IS THE WT. PERCENT OF THE ORIGINAL COAL THAT IS NOW	C 1250
C	VOLATILIZED CARBON.	C 1260
C	CHARC IS THE PERCENTAGE OF THE ORIGINAL COAL THAT NOW CONSISTS	C 1270
C	OF CHAR CARBON.	C 1280
C	FRAC IS THE MASS FRACTION OF CARBON IN THE CHAR.	C 1290
C	MOLUC AND MOLCC ARE MOLAR FLOWRATES OF VOLATILE AND CHAR	C 1300
C	CARBON IN LBMOL/HR.	C 1310
C		C 1320
	GO TO 103	C 1330
102	CONTINUE	C 1340
C		C 1350
C	NOT ENOUGH VOLATILES WERE PRODUCED TO LEAVE ONLY CARBON AND	C 1360
C	ASH IN THE CHAR.	C 1370
C		C 1380
	VOLMIN=(HY+NI+SU+OX+WATER)/100.	C 1390
	WRITE (6,104) VOLMIN,FUL	C 1400
C		C 1410
C	THE VOLATILES FRACTION IS ARBITRARILY INCREASED TO VOLMIN.	C 1420
C		C 1430
	CARBOL=0.	C 1440
	UCARB=0.	C 1450
	CHARC=CARB	C 1460
	FRAC=CHARC/(CHARC+ASH)	C 1470
	MOLUC=0.	C 1480
	MOLCC=CHARC*FLOCOL/1200.	C 1490
103	CONTINUE	C 1500
C		C 1510
C	FIND FLOWRATES OF THE PRODUCTS OF VOLATILES COMBUSTION IN LBMOL/HR	C 1520
C	NITROGEN FLOWRATE IS UNCHANGED.	C 1530
C		C 1540
	CO2=0.	C 1550
	H2=CO2	C 1560
	CO=MOLUC	C 1570
	H2O=MOLH/2+MOLWTR	C 1580
	NO=MOLN	C 1590
	SO2=MOLS	C 1600
	UX2=MOL02-.5*(CO+MOLH/2.+NO-MOLO)-SO2	C 1610
	HRPYR2=FLOCOL*(CHV-(1.-FUL)*FRAC*14110.)-CO*121750.	C 1620
C		C 1630
C	HEAT RELEASE THROUGH VOLATILES COMBUSTION IN BTU/HR.	C 1640
C	NOW FIND THE INPUT ENTHALPY OF THE REACTANTS IN BTU/HR RELATIVE	C 1650
C	TO A REFERENCE TEMPERATURE OF 500 R.	C 1660
C		C 1670
	TR=500.	C 1680
	HPRI=6.557*(TPRI-TR)+.0004103*(TPRI**2-TR**2)-2.21E-8*(TPRI**3-TR*	C 1690
	1*3)	C 1700
	HSEC=6.557*(TSEC-TR)+.0004103*(TSEC**2-TR**2)-2.21E-8*(TSEC**3-TR*	C 1710
	1*3)	C 1720
	HCOAL=.3*(TPRI-TR)	C 1730
	HREACT=HPRI*FLOPRI/23.+HSEC*FLOSEC/29.+HCOAL*FLOCOL	C 1740
C		C 1750
C	TOTAL ENTHALPY EQUALS HRPYR2 + HREACT.	C 1760
C		C 1770
	HTPYR2=HRPYR2+HREACT	C 1780

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      FVOL=FUL
      WRITE (6,106) CO,CO2,H2,H2O,NO,MOLN2,OX2,S02,PMAS,FRAC,FUL,HRPYR2
      RETURN
C
104 FORMAT (/,10X, 26HNOT ENOUGH VOLATILES WERE , 36HPRODUCED TO LEAVE
1 ONLY CARBON AND ASH , 12HIN THE CHAR.,/,10X, 12HTHE MINIMUM , 37H
2VOLATILES MASS FRACTION NECESSARY IS ,E12.4, 34H LE VOLATILES/LB A
3S-RECEIVED COAL.,/,10X, 35HTHE ACTUAL VOLATILES MASS FRACTION . 4
4HMAS ,E12.4,/)
105 FORMAT (////,10X, 36H*** FINAL PYROLYSIS CALCULATIONS ***,/)
106 FORMAT (1X, 28HGAS FLOWRATES, LBMOL/HR. , 41HAFTER PYROLYSIS AND
1VOLATILES COMBUSTION-/,1X, 38HCO, CO2, H2, H2O, NO, N2, O2, AND S
2O2.,/,10X,8E12.3,/,1X, 22HCHAR FLOWRATE, LB/HR. , 30HAND CHAR CAR
3BON MASS FRACTION.,/,10X,2E12.3,/,1X, 24HVOLATILES MASS FRACTION
4, 40HAND HEAT RELEASE VIA VOLATILES BURNING, , 7HBTU/HR.,/,10X,2E
512.3,/)
C
      END
      SUBROUTINE RUNPT (PTMP,PTMP2,DIA,DENCIL,TF,TPYR2,DT,KGAS)
      REAL KGAS
C
      THIS SUBROUTINE USES A PUNGE-KUTTA METHOD TO INTEGRATE THE
C      PARTICLE TEMPERATURE VERSUS TIME EXPRESSION.
C
      Y1=DT*FPT(DIA,DENCIL,TF,PTMP,KGAS,TPYR2)
      PT2=PTMP+.5*Y1
      Y2=DT*FPT(DIA,DENCIL,TF,PT2,KGAS,TPYR2)
      PT3=PTMP+.5*Y2
      Y3=DT*FPT(DIA,DENCIL,TF,PT3,KGAS,TPYR2)
      PT4=PTMP+Y3
      Y4=DT*FPT(DIA,DENCIL,TF,PT4,KGAS,TPYR2)
      DPT=(Y1+2.*(Y2+Y3)+Y4)/6.
      PTMP2=PTMP+DPT
      RETURN
C
      END
      FUNCTION FPT(DIA,DENCIL,TF,PT,KGAS,TPYR2)
      REAL KGAS
C
      THIS SUBPROGRAM IS USED WITH SUBROUTINE RUNPT TO FIND
C      THE PARTICLE TEMPERATURE AS A FUNCTION OF TIME.
C
      PMASS=DENCIL*3.14159*DIA**3/6.
      A=3.14159*DIA**2
      H=4.*KGAS/DIA
      SB=1.714E-9
      EPS=1.
      CP=.3
      FPT=A*(EPS*SB*(.5*(TF-50.))**4+.5*TF**4-PT**4)+H*(TPYR2-PT))/(PMASS
1*CP*3600.)
C
      FPT IS THE PARTICLE HEATING RATE IN DEGREES RANKINE PER SECOND.
C
      RETURN
C
      END
      SUBROUTINE PSR (DCRITM,BURNT,BURN,MOUTT,CO,H2O,NO,S02,O2,N2,HTOT1,
1FRAC,TF,GLOSS,TFNEW,MCO,MCO2,M02,HTOT2,CHV,X0,ALPHA,H2)
      EXTERNAL FCN
      REAL MOUT,MBURN,MBURNT,MOUTT,MCO,MH2O,M02,MCO2,NO,N2

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	COMMON /A/ IFLAG	F	50
	COMMON /B/ DCAR, S, EXPAN, FLOCOL, FVOL, CL, CR, TR, TL, EXAIR, RCRT	F	60
	COMMON /D/ KFLAG	F	70
	COMMON /F/ TF2, GMD02, GMCO2, GH2, MH2O, GNO, GN2, GMD2, GSO2, TMOLES	F	80
	COMMON /G/ GASIND	F	90
	DIMENSION SIZE(100), MOUT(100)	F	100
	DIMENSION XO(5), ALPHA(5)	F	110
	WRITE (6,110)	F	120
	IF (KFLAG.EQ.0) H2=0.	F	130
	MOUTT=0.0	F	140
	BURNT=0.0	F	150
	BURN=0.0	F	160
	STEP=0.10	F	170
C		F	180
C	CALCULATE PARTICLE SIZE DISTRIBUTION AFTER DEVOLATILIZATION	F	190
C	PARTICLE SIZE DISTRIBUTION IS BROKEN INTO 100 PORTIONS	F	200
C		F	210
	DO 101 I=1,100	F	220
	RR=100.5-FLOAT(I)	F	230
	CHARIN=FLOCOL*(1.-FVOL)	F	240
	SIZE(I)=(DCAR*(ALOG(100./RR))**((1./S))*EXPAN**3	F	250
C		F	260
C	CALC QUANTITIES OF CHAR BURNT AND PASSED	F	270
C		F	280
	MOUT(I)=CHARIN*.010*(DCRITH/SIZE(I))**3	F	290
	IF (SIZE(I).LE.DCRITH) MOUT(I)=0.0	F	300
	MBURNT=.010*(FLOCOL-MOUT(I))	F	310
	MBURN=.010*(CHARIN-MOUT(I))	F	320
	BURNT=BURNT+MBURNT	F	330
	BURN=BURN+MBURN	F	340
	MOUTT=MOUTT+MOUT(I)	F	350
C		F	360
C	RR - ROSIN RAMMLER SIZE PARAMETER, CHARIN - CHAR INTO PSR, LB/HR.	F	370
C	SIZE(I) - INPUT SIZES OF CHAR PARTICLES, MICRONS,	F	380
C	MOUTT, MOUT(I) - MASS FLOW OF PARTICLES OUT OF PSR, LB/HR,	F	390
C	MBURNT - TOTAL COAL BURNT, LB/HR, MBURN - TOTAL CHAR BURNT, LB/HR,	F	400
C	BURNT, BURN - RESPECTIVE TOTALS OVER LOOP ITERATIONS, LB/HR.	F	410
C	CALC CARBON MOLES BURNT IN PSR	F	420
C		F	430
	101 CONTINUE	F	440
	OUTC=FRAC*MOUTT/12.	F	450
	RCU=FRAC*(CHARIN-MOUTT)/12.	F	460
	PSRV=(CL-TL)*3.14159*(CR**2-RCRT**2)	F	470
	CHRBRN=CHARIN-MOUTT	F	480
	CARBIN=FRAC*CHARIN/12.	F	490
C		F	500
C	OUTC - CARBON FLOW OUT OF PSR, LB-MOLES/HR.	F	510
C	RCU - CARBON BURNED IN PSR, LB-MOLES/HR.	F	520
C	PSRV - PSR VOLUME, FT2.	F	530
C	CALC EXTENT OF CO TO CO2 CONVERSION	F	540
C		F	550
	WRITE (6,111) PSRV,CARBIN,CHARIN,RCU,CHRBRN,OUTC,MOUTT	F	560
	WRITE (6,112)	F	570
	IF ((RCU+.5*CO).GT.02) WRITE (6,113)	F	580
C		F	590
C	CHECK IF FUEL RICH OR AIR RICH	F	600
C	TWO SEPERATE PROCEDURES ARE USED DEPENDING ON STOICHIOMETRY, IN	F	610
C	ORDER TO SPEED CONVERGENCE	F	620
C		F	630
	IF ((RCU+.5*CO).LT.02) GO TO 104	F	640

	GASIND=RCU-2.*O2	F 650
	IF (GASIND.LT.0.) GO TO 102	F 660
C		F 670
C	THERE IS NOT ENOUGH OXYGEN TO BURN ALL THE RELEASED CARBON	F 680
C	TO CO. PERFORM A GASIFICATION ANALYSIS.	F 690
C	THE AMOUNT OF CARBON BURNED IS LIMITED BY THE OXYGEN FLOWRATE.	F 700
C		F 710
	RCU=2.*O2	F 720
	MOUTT=CHARIN-12.*RCU/FRAC	F 730
	OUTC=FRAC*MOUTT/12.	F 740
	CHRBRN=CHARIN-MOUTT	F 750
C		F 760
C	FORMULATE INITIAL GUESSES FOR SUBROUTINE EQLBRM.	F 770
C		F 780
	M02=0.	F 790
	MH2O=.5*M2O	F 800
	H2=.5*M2O	F 810
	MCO2=.5*M2O	F 820
	MCO=CO+RCU-MCO2	F 830
	TMOLES=M02+MCO+MCO2+MH2O+H2+N2+NO+S02	F 840
C		F 850
C	CALCULATE HEAT RELEASE.	F 860
C		F 870
	HREACT=RCU*(12.*14110.-121750.)	F 880
	HTOT2=HTOT1+HREACT-QLOSS	F 890
	CAREFF=(MCO+MCO2)/(MCO+MCO2+OUTC)	F 900
	WRITE (6,109)	F 910
	WRITE (6,111) PSRU,CARBIN,CHARIN,RCU,CHRBRN,OUTC,MOUTT	F 920
	WRITE (6,116)	F 930
C		F 940
C	PERFORM THE EQUILIBRIUM ANALYSIS.	F 950
C		F 960
	CALL EQLBRM (MOUTT,HTOT2,TF,TFNEW,X0,ALPHA,JFLAG,MCO,MCO2,H2,MH2O,	F 970
	INO,N2,M02,S02,TMOLES)	F 980
	IF (IFLAG.EQ.1) TFNEW=TF	F 990
	TF2=TFNEW	F 1000
	GMCO=MCO	F 1010
	GMC02=MCO2	F 1020
	GH2=H2	F 1030
	GNO=NO	F 1040
	GN2=N2	F 1050
	GM02=M02	F 1060
	GS02=S02	F 1070
C		F 1080
C	CALCULATE THE GASIFICATION PARAMETERS.	F 1090
C		F 1100
	CALL GASPAR (CHU,FLOCOL,EXAIR)	F 1110
	WRITE (6,118) CAREFF	F 1120
	RETURN	F 1130
102	N=0	F 1140
	MH2O=H2O	F 1150
	MCO=2.0*(RCU-O2)+CO	F 1160
C		F 1170
C	LOOP FOR SUBSTOICHIOMETRIC CASES	F 1180
C		F 1190
103	MCO=(1.000+STEP)*MCO	F 1200
	MCO2=CO+RCU-MCO	F 1210
	M02=O2-0.5*(RCU+MCO2)	F 1220
	N=N+1	F 1230
	TMOLES=MCO+MH2O+NO+S02+N2+M02+MCO2	F 1240

	FCO=MCO/TMOLES	F 1250
	FH2O=MH2O/TMOLES	F 1260
	F02=M02/TMOLES	F 1270
	P=1.00	F 1280
	TC=P/(TF*0.730)	F 1290
C		F 1300
C	CALC CONCENTRATIONS OF CO, H2O, O2, IN LB MOLES/FT**3	F 1310
C		F 1320
	CONCO=TC*FCO	F 1330
	CONH2O=TC*FH2O	F 1340
	CONO2=TC*F02	F 1350
	RR=7.497E+15*(CONH2O**0.5)*(CONO2**0.5)*EXP(-53964./(TF*1.986))	F 1360
	RCO=CONCO*RR	F 1370
	CORES=MCO-(CO+RCU-RCO*PSRV)	F 1380
C		F 1390
C	MCO, MCO2, M02, MH2O, N2, NO, SO2 - MOLAR FLOW OF GASES, LB-MOLES/	F 1400
C	CONCO, CONH2O, CONO2 - GAS CONCENTRATIONS LB-MOLES/FT3,	F 1410
C	RCO- REACTION RATE OF CO DEPLETION (CO2 FORMATION), LB-MOLES/FT3-H	F 1420
C	CORES - RESIDUAL CONCENTRATION OF CO TO TEST FOR CLOSEST SOLUTION.	F 1430
C		F 1440
	WRITE (6,114) N,MCO,MCO2,M02,TMOLES,CONH2O,CONO2,RCO	F 1450
C		F 1460
C	APPROPRIATE STEP SIZE IS CHOSEN	F 1470
C		F 1480
	IF (CORES.GT.0.0.AND.N.LT.10) STEP=STEP/10.	F 1490
	IF (CORES.GT.0.0.AND.N.LT.10) GO TO 102	F 1500
	IF (CORES.GT.0.0) GO TO 106	F 1510
	IF (N.GT.200) WRITE (6,115)	F 1520
	IF (N.GT.200) STOP	F 1530
	GO TO 103	F 1540
104	CONTINUE	F 1550
	N=0	F 1560
C		F 1570
C	INITIALIZE QUANTITIES TO BEGIN ITERATIVE SOLUTION	F 1580
C		F 1590
	MCO=0.0001*CO	F 1600
	MH2O=H2O	F 1610
	MCO2=CO+RCU-MCO	F 1620
	M02=O2-0.5*(RCU+MCO2)	F 1630
C		F 1640
C	LOOP FOR AIR RICH CASES	F 1650
C	SEE COMMENTS IN SUBSTOICHIOMETRIC LOOP	F 1660
C	CALC MOLE FRACTIONS OF CO, H2O, AND O2	F 1670
C		F 1680
105	CONTINUE	F 1690
	N=N+1	F 1700
	TMOLES=MCO+MH2O+NO+SO2+N2+M02+MCO2	F 1710
	FCO=MCO/TMOLES	F 1720
	FH2O=MH2O/TMOLES	F 1730
	F02=M02/TMOLES	F 1740
C		F 1750
C	CALC CONCENTRATIONS OF CO, H2O, O2, IN LB MOLES/FT**3	F 1760
C		F 1770
	P=1.00	F 1780
	TC=P/(TF*0.730)	F 1790
	CONCO=TC*FCO	F 1800
	CONH2O=TC*FH2O	F 1810
	CONO2=TC*F02	F 1820
C		F 1830
C	CALC RCO	F 1840

C	RR=7.497E+15*(CONH2O**0.5)*(CONO2**0.5)*EXP(-53964./(TF*1.986))	F 1850
	RCO=CONCO*RR	F 1860
C		F 1870
C	CALC FLOWS OUT OF PSR	F 1880
C	CO OUT OF PSR IS CALCULATED FROM REARRANGED PSR EQUATION	F 1890
C		F 1900
	XCO=MCO	F 1910
	MCO=(CO+RCU)/(1.0+RR*TC*PSRU/TMOLES)	F 1920
	MCO2=CO+RCU-MCO	F 1930
	MO2=O2-.5*(RCU+MCO2)	F 1940
	WRITE (6,114) N,MCO,MCO2,MO2,TMOLES,CONH2O,CONO2,RCO	F 1950
	IF (N.GT.25) WRITE (6,115)	F 1960
	IF (N.GT.25) GO TO 106	F 1970
	IF (ABS(1.-XCO/MCO).LT..001) GO TO 106	F 1980
	GO TO 105	F 1990
106	CONTINUE	F 2000
	H2=0.	F 2010
	TMOLES=MCO+MCO2+MH2O+NO+N2+MO2+SO2+H2	F 2020
	WRITE (6,116)	F 2030
		F 2040
C	FLAG = 1.0 FOR FIXED TEMP CALCULATIONS	F 2050
C		F 2060
C	IF (IFLAG.EQ.1) TFNEW=TF	F 2070
	IF (IFLAG.EQ.1) WRITE (6,117) MH2O,MCO,N2,MO2,MCO2,NO,SO2,H2,MOUTT	F 2080
	1,TFNEW,OUTC	F 2090
	IF (KFLAG.EQ.0) GO TO 107	F 2100
		F 2110
C		F 2120
C	CHECK THE KINETIC RESULTS AGAINST EQUILIBRIUM LIMITATIONS.	F 2130
C	IF JFLAG EQUALS ONE THE KINETIC RESULTS ARE IN VIOLATION.	F 2140
		F 2150
	IF (IFLAG.EQ.1) CALL EQLBRM (MOUTT,HTOT2,TF,TFNEW,X0,ALPHA,JFLAG,M	F 2160
	1CO,MCO2,H2,MH2O,NO,N2,MU2,SO2,TMOLES)	F 2170
	IF (IFLAG.EQ.1.AND.JFLAG.EQ.1) WRITE (6,120)	F 2180
107	CONTINUE	F 2190
	IF (IFLAG.EQ.1) GO TO 108	F 2200
		F 2210
C		F 2220
C	CALC PSR TEMPERATURE	F 2230
C	HREACT - CHEMICAL HEAT GENERATION BTU/HR	F 2240
		F 2250
	HREACT=RCU*(12.*14110.-121750.)+MCO2*121750.	F 2260
	HTOT2=HTOT1+HREACT-QLOSS	F 2270
C		F 2280
C	TOTAL ENTHALPY OF FLOW RELATIVE TO REFERENCE TEMP	F 2290
C		F 2300
	CALL TEMP (MCO,MCO2,H2,MH2O,NO,N2,MO2,SO2,MOUTT,HTOT2,500.,3000.,T	F 2310
	1FNEW)	F 2320
	WRITE (6,117) MH2O,MCO,N2,MO2,MCO2,NO,SO2,H2,MOUTT,TFNEW,OUTC	F 2330
	IF (KFLAG.EQ.0) GO TO 108	F 2340
	CALL EQLBRM (MOUTT,HTOT2,TFNEW,TFNEW,X0,ALPHA,JFLAG,MCO,MCO2,H2,MH	F 2350
	12O,NO,N2,MO2,SO2,TMOLES)	F 2360
	IF (JFLAG.EQ.1) WRITE (6,121)	F 2370
108	CONTINUE	F 2380
	CAREFF=(MCO+MCO2)/(MCO+MCO2+OUTC)	F 2390
		F 2400
C	CAREFF - CARBON EFFICIENCY	F 2410
C		F 2420
C	WRITE (6,118) CAREFF	F 2430
	WRITE (6,119) TFNEW,TF	F 2440
	RETURN	

C	109	FORMAT (/,10X, 34HGASIFICATION RUN-REVISED BURN DATA,/) F	2450
	110	FORMAT (///,10X, 24H*** PSR CALCULATIONS.***,/) F	2460
	111	FORMAT (/,12X, 13HPSR VOLUME = ,E12.4, 6H FT**3,/,12X, 48HPSR BU F	2470
		1RN DATA-CARBON IN LBMOLE/HR, CHAR IN LB/HR,/,30X, 16HCARBON C	2480
		2HAR,/,12X, 16HFLOW INTO PSR ,2E12.4,/,12X, 16HBURNED IN PSR , F	2490
		32E12.4,/,12X, 16HFLOW OUT OF PSR ,2E12.4,/) F	2500
	112	FORMAT (/,12X, 29HINTERMEDIATE VALUES-FLOWS IN , 43HLBMOLE/HR, CON F	2510
		1CENTRATIONS IN LBMOLE/FT**3, , 29HCO BURNUP IN LBMOLE/HR FT**3,/, F	2520
		212X, 48HTRIAL CO FLOW CO2 FLOW O2 FLOW , 48HTOTAL F	2530
		3 FLOW H2O CONC. O2 CONC. CO BURNUP,/) F	2540
	113	FORMAT (1X,17HSUBSTOICHIOMETRIC) F	2550
	114	FORMAT (12X,13,9X,7E12.4) F	2560
	115	FORMAT (10X,21HPSR WILL NOT CONVERGE) F	2570
	116	FORMAT (///,12X, 25HOUTLET FLOWRATES-GAS AND , 42HCARBON FLOWS IN L F	2580
		1BMOLE/HR, CHAR IN LB/HR, , 9HTEMP IN R,/,12X, 30HFH2O FCO F	2590
		2 FN2 , 50HF02 FCO2 FNO FS02 FH2 F	2600
		3 , 26HCHAR TEMP CARBON,/) F	2610
	117	FORMAT (1X, 8HKINETIC ,11E10.3) F	2620
	118	FORMAT (/,1X,22HPSR CARBON EFFICIENCY=,F10.6) F	2630
	119	FORMAT (1X, 24HNEW FLAME TEMPERATURE = ,F10.2, 26H OLD FLAME TEMP F	2640
		1ERATURE = ,F10.2,/) F	2650
	120	FORMAT (10X, 30HTHE PSR CO2/CO RATIO EXCEEDED , 44HTHE EQUILIBRIUM F	2660
		1 VALUE OR OXYGEN IS DEPLETED,/,10X, 46HEQUILIBRIUM MOLE FRACTIONS F	2670
		2 ARE NOW BEING USED.) F	2680
	121	FORMAT (10X, 51HTHE PSR TEMPERATURE EXCEEDED THE EQUILIBRIUM VALUE F	2690
		1,/,10X, 51HEQUILIBRIUM MOLE FRACTIONS AND TEMPERATURE ARE NOW , 1 F	2700
		21HBEING USED.) F	2710
		F	2720
		F	2730
		F	2740
	END		
	SUBROUTINE PFR (DCRIT,RCRIT,L,TROR,DENCOL,FRAC,H2O,CO,N2,O2,CO2,NO	G	10
	1,S02,TPSR,CHAR,HINFUT,TROL,CHU,X0,ALPHA,H2)	G	20
		C	30
C	N2, O2, H2O, CO, CO2, NO, S02, FLOWS IN LB-MOLES HR, CHAR-LB/HR.	G	40
C		G	50
C	EXTERNAL FCN	G	60
	COMMON /A/ IFLAG	G	70
	COMMON /D/ KFLAG	G	80
	COMMON /F/ TOUT,FCO,FCO2,FH2,FH2O,FNO,FN2,F02,FS02,MOLFLO	G	90
	COMMON /H/ EXAIR2,FLOCL2	G	100
	DIMENSION X0(5), ALPHA(5)	G	110
	DIMENSION SIZE(10), FCHAR(10)	G	120
	REAL KES,KD,NEWCO,NEWCO2,MOLFLO,N2,NO,L	G	130
	WRITE (6,109)	G	140
	DHR=0.0	G	150
	PI=3.14159	G	160
	T=TPSR	G	170
	DIA=DCRIT/304800.	G	180
	WRITE (6,110)	G	190
	M=10	G	200
	D=10.	G	210
	C=0.0	G	220
	AREA=PI*TROR**2	G	230
C		G	240
C	AREA - THROAT AREA, FT2.	G	250
C		G	260
	FCO=0.	G	270
	FCO2=0.	G	280
	FH2=0.	G	290
	FH2O=0.	G	300

	F02=0.	G	310
	FH=0.	G	320
	KK=20	G	330
	XK=20.	G	340
	DX=(L-TROL)/(D*XK)	G	350
	X=DX	G	360
	M=1	G	370
C		G	380
C	LOOP OVER PLUG FLOW REACTOR LENGTH	G	390
C		G	400
101	CONTINUE	G	410
	IF (X.GT.L-TROL) GO TO 102	G	420
	C=C+1.	G	430
	FCO=FCO+CO/D	G	440
	FCO2=FCO2+CO2/D	G	450
	F02=F02+O2/D	G	460
	FH2O=FH2O+H2O/D	G	470
	FH2=FH2+H2/D	G	480
	FN2=FN2+C/D	G	490
	FNO=FNO+C/D	G	500
	FSO2=SO2*C/D	G	510
	FH=FH+HINPUT/D	G	520
C		G	530
C	FLows INTO EACH REACTOR SECTION, LB-MOLes/HR.	G	540
C		G	550
	FCHAR(N)=CHAR/D	G	560
	SIZE(N)=DIA	G	570
102	CONTINUE	G	580
	MOLFLO=FH2O+FCO+FN2+F02+FCO2+FNO+FSO2	G	590
	VOLFLO=MOLFLO*T*.730	G	600
	VEL=VOLFL0/AREA	G	610
	KES=11.97*T*EXP(-14492./T)	G	620
	TC=1.0/(T*.730)	G	630
	DT=DX/VEL	G	640
	DVOL=AREA*DX	G	650
C		G	660
C	MOLFLO, VOLFL0 - TOTAL MOLAR FLOWRATE OF GAS, LB-MOLes/HR AND VOLU	G	670
C	FLOW, FT3/HR.	G	680
C	VEL - GAS VELOCITY FT/HR, KES - CHAR CHEMICAL RATE CONSTANT,	G	690
C	LB CARBON-FT/LB-MOLes O2-S, TC - GAS CONCENTRATION, LB-MOLes/FT3,	G	700
C	FCHAR(N) - FLOW OF CHAR OF SIZE N, LB/HR, SIZE(N) - DIAMETER OF	G	710
C	PARTICLE, FT, DX - INCREMENT OF PFR LENGTH, FT, DT - GAS RESIDENC	G	720
C	TIME IN PFR SEGMENT, HR, DVOL - VOLUME OF PFR SEGMENT FT3.	G	730
C	LOOP OVER SMALLEST REACTOR LENGTH SEGMENTS	G	740
C		G	750
	DO 104 K=1, KK	G	760
	X=X+DX	G	770
	IF (X.GT.L+.4) GO TO 102	G	780
C		G	790
C	BEGIN LOOP OVER PARTICLE SIZES	G	800
C		G	810
	DO 103 J=1, N	G	820
	CONCO2=TC*F02/MOLFLO	G	830
	CONH2O=TC*FH2O/MOLFLO	G	840
	CONCO=TC*FCO/MOLFLO	G	850
	KD=1.5*0.1078*T/(2700.*SIZE(J))	G	860
	PCHAR=(1./(1./KES+1./KD))*CONCO2/FRAC	G	870
	SPA=6./(DENCO*SIZE(J))	G	880
	PAREA=SPA*FCHAR(J)*DT	G	890
	REACT=RCHAR*PAREA*2600.	G	900

	IF (REACT.GE.FCHAR(J)) REACT=FCHAR(J)	G 910
	NEWCO=REACT*FRAC/12.0	G 920
	RCO=7.497E+15*(CONCO)*(CONH2O**0.5)*(CONO2**0.5)*EXP(-53964./	G 930
1	/(T*1.986))	G 940
	NEWCO2=RCO*DVOL	G 950
C		G 960
C	CONO2, CONH2O, CONCO - GAS CONCENTRATIONS LB-MOLES/FT3, KD - CHAR	G 970
C	DIFFUSION RATE COEFFICIENT, LB CARBON-FT/LB-MOLES O2-S	G 980
C	RCHAR - REACTION RATE FOR CHAR, LB-CHAR/FT2-S, SPA - SPECIFIC ARE	G 990
C	OF CHAR, FT2/LB, PAREA - TOTAL PARTICLE AREA EXPOSED IN PFR SEGME	G 1000
C	FT2, REACT - CHAR REACTION RATE, LB-CHAR/HR, NEWCO - CO GENERATE	G 1010
C	LB-MOLES/HR, RCO - CO CONVERSION RATE, LB-MOLES CO/FT3-HR,	G 1020
C	NEWCO2 - CO2 GENERATED, LB-MOLES/HR.	G 1030
C		G 1040
	IF (NEWCO2.GT.FCO) NEWCO2=FCO	G 1050
	DO2=0.5*(NEWCO2+NEWCO)	G 1060
	IF (DO2.GT.FO2) WRITE (6,111)	G 1070
	IF (DO2.GT.FO2) X=X+(20.0-FLOAT(K))*DX	G 1080
	IF (DO2.GT.FO2) GO TO 105	G 1090
	FCO2=FCO2+NEWCO2	G 1100
	FCO=FCO+NEWCO-NEWCO2	G 1110
	FO2=FO2-DO2	G 1120
	FH=FH+(FRAC*REACT/12.)*(12.*14110.-121750.)+NEWCO2*121750.	G 1130
	SIZE(J)=SIZE(J)*((FCHAR(J)-REACT)/FCHAR(J))*((1./3.))	G 1140
	FCHAR(J)=FCHAR(J)-REACT	G 1150
103	CONTINUE	G 1160
104	CONTINUE	G 1170
105	TCHAR=0.0	G 1180
	DO 106 I=1,N	G 1190
106	TCHAR=TCHAR+FCHAR(I)	G 1200
C		G 1210
C	FLAG = 1.0 FOR ISOTHERMAL CASE	G 1220
C		G 1230
	MOLFLO=FCO+FCO2+FH2+FH2O+FNO+FN2+FO2+FSO2	G 1240
	IF (IFLAG.EQ.1) TOUT=T	G 1250
	WRITE (6,112) FH2O,FCO,FN2,FO2,FCO2,FNO,FSO2,FH2,TCHAR,TOUT,X	G 1260
	IF (IFLAG.EQ.1.AND.KFLAG.EQ.0) GO TO 107	G 1270
C		G 1280
C	CHECK THE KINETIC RESULTS AGAINST THE EQUILIBRIUM LIMITATIONS.	G 1290
C		G 1300
	IF (IFLAG.EQ.1.AND.KFLAG.EQ.1) CALL EQLBRM (TCHAR,FH,T,TOUT,XO,ALP	G 1310
	1HA,JFLAG,FCO,FCO2,FH2,FH2O,FNO,FN2,FO2,FSO2,MOLFLO)	G 1320
	IF (IFLAG.EQ.1.AND.KFLAG.EQ.1.AND.JFLAG.EQ.1) WRITE (6,114) X	G 1330
	IF (IFLAG.EQ.1) GO TO 107	G 1340
	CALL TEMP (FCO,FCO2,FH2,FH2O,FNO,FN2,FO2,FSO2,TCHAR,FH,500.,T,TOUT	G 1350
	1)	G 1360
	T=TOUT	G 1370
	IF (KFLAG.NE.1) GO TO 107	G 1380
	CALL EQLBRM (TCHAR,FH,T,TOUT,XO,ALPHA,JFLAG,FCO,FCO2,FH2,FH2O,FNO,	G 1390
	1FN2,FO2,FSO2,MOLFLO)	G 1400
	IF (JFLAG.EQ.1) WRITE (6,115) X	G 1410
107	CONTINUE	G 1420
	N=N+1	G 1430
	IF (N.GT.10) N=10	G 1440
	GO TO 101	G 1450
108	CEFF=(FCO+FCO2)/(FCO+FCO2+(TCHAR*FRAC/12.))	G 1460
	WRITE (6,113) FCO,FCO2,FO2,TCHAR,TOUT,CEFF	G 1470
	IF (EXAIR2.LT.1.) CALL GASPAR (CHU,FLUCL2,EXAIR2)	G 1480
	RETURN	G 1490
C		G 1500

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109 FORMAT (///,10X,30H*** PLUG FLOW CALCULATIONS ***) G 1510
110 FORMAT (///,12X, 29HGAS FLOWS IN LBMOLE/HR, CHAR , 30HIN LB/HR, TEM G 1520
1P IN R, X IN FEET,/,12X, 40HFH2O FCO FN2 F02 G 1530
2 , 40HFCO2 FNO FSO2 FH2 , 21HCHAR TEMP G 1540
3 X,/) G 1550
111 FORMAT (1X,21H** OXYGEN DEPLETED **) G 1560
112 FORMAT (/,1X, 8HKINETIC ,11E10.3) G 1570
113 FORMAT (///,1X,16HFINAL FLOWS CO=,F10.6,3X,4HCO2=,F10.6,3X,3HO2=,F G 1580
110.6,3X,5HCHAR=,F10.6,3X,5HTEMP=,F8.2,3X,5HCEFF=,F8.5) G 1590
114 FORMAT (10X, 7HAT X = ,F7.3, 9H FEET IN , 34HTHE PFR THE CO2/CO G 1600
1RATIO EXCEEDED , 46HTHE EQUILIBRIUM VALUE, OR OXYGEN WAS DEPLETED. G 1610
2,/,10X, 46HEQUILIBRIUM MOLE FRACTIONS ARE NOW BEING USED.) G 1620
115 FORMAT (10X, 7HAT X = ,F7.3, 9H FEET IN , 55HTHE PFR THE TEMPERA G 1630
1TURE EXCEEDED THE EQUILIBRIUM VALUE,/,10X, 51HEQUILIBRIUM MOLE FR G 1640
2ACTIONS AND TEMPERATURE ARE NOW , 11HBEING USED.) G 1650
C G 1660
END G 1670
SUBROUTINE TEMP (CO,CO2,H2,H2O,NO,N2,O2,SO2,CASH,DELTAH,TR,TI,T) H 10
REAL N2,NO H 20
T=TI H 30
II=0 H 40
101 CONTINUE H 50
II=II+1 H 60
IF (II.GT.100) WRITE (6,103) H 70
IF (II.GT.100) GO TO 102 H 80
C H 90
C CALC ENTHALPY CHANGE H 100
C H 110
DT=T-TR H 120
DTIN=1./T-1./TR H 130
TRA=T/TR H 140
C H 150
C INTEGRATED SPECIFIC HEAT EQUATIONS FOR H2O, CO, N2, O2, CO2 (WARK) H 160
C H 170
DH2=5.76*DT+.000229*(T**2-TR**2)+40.*(T**.5-TR**.5) H 180
DH2O=19.86*DT-1194.*(T**.5-TR**.5)+7500.*ALOG(TRA) H 190
DHCO=9.46*DT-3290.*ALOG(TRA)-1.07E+6*DTIN H 200
DHN2=9.47*DT-3470.*ALOG(TRA)-1.16E+6*DTIN H 210
DHO2=11.515*DT-344.*(T**.5-TR**.5)+1530.*ALOG(TRA) H 220
DHCO2=16.20*DT-6530.*ALOG(TRA)-1.41E+6*DTIN H 230
DHCASH=0.30*DT H 240
HNEW=DH2O*H2O+DHCO*(CO+NO)+DHN2*N2+DHO2*O2+DHCO2*(CO2+SO2)+DHCASH H 250
1*CASH+DH2*H2 H 260
HDIFF=DELTAH-HNEW H 270
C H 280
C HNEW - NEW ENTHALPY FLOW BASED ON T, BTU/HR, HDIFF - RESIDUAL H 290
C ENTHALPY FLOW VALUE, BTU/HR H 300
C VALUE, BTU/HR. H 310
C CALC NEW TEMPERATURE T AND ITERATE H 320
C H 330
T=T+HDIFF*T/DELTAH H 340
IF (T.LT.0.) T=600. H 350
C H 360
C CHECK FOR SOLUTION CONVERGENCE H 370
C H 380
IF (ABS(HDIFF/DELTAH).LT..0002) GO TO 102 H 390
GO TO 101 H 400
102 RETURN H 410
C H 420
103 FORMAT (1X,17HDOES NOT CONVERGE) H 430

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C	END	H	440
	SUBROUTINE EQLBRM (TCHAR,FH,T,TOUT,X0,ALPHA,JFLAG,FCO,FCO2,FH2,FH2	H	450
	10,FNO,FN2,F02,FSO2,MOLFLO)	I	10
	EXTERNAL FCN	I	20
	DIMENSION X0(5), ALPHA(5)	I	30
	COMMON /A/ IFLAG	I	40
	COMMON /D/ KFLAG	I	50
	COMMON /E/ KP1,KP2,FFFCO,FFFCO2,FFFH2,FFFH2O,FFFN0,FFFN2,FFFO2,FFF	I	60
	1SO2	I	70
	COMMON /UNITS/ NUNITS	I	80
	REAL KP1,KP2,MOLFLO	I	90
C		I	100
C	THIS SUBROUTINE COMPUTES GAS COMPOSITION AND TEMPERATURE BASED	I	110
C	ON AN EQUILIBRIUM MODEL.	I	120
C		I	130
	FFFCO=FCO	I	140
	FFFCO2=FCO2	I	150
	FFFH2=FH2	I	160
	FFFH2O=FH2O	I	170
	FFFN0=FNO	I	180
	FFFN2=FN2	I	190
	FFFO2=F02	I	200
	FFFSO2=FSO2	I	210
	FFFFLO=MOLFLO	I	220
	TRIALT=T	I	230
	KOUNT=0	I	240
101	CONTINUE	I	250
	KOUNT=KOUNT+1	I	260
	IF (KOUNT.GT.25) GO TO 107	I	270
C		I	280
C	FIRST CALCULATE TWO EQUILIBRIUM CONSTANTS AT TEMPERATURE TRIALT.	I	290
C	THE FIRST IS FOR CO2 = CO + .5*O2.	I	300
C		I	310
	CLOG1=(-6.94E-7)*TRIALT**2+(7.074E-3)*TRIALT-19.3565	I	320
	KP1=10.**CLOG1	I	330
C		I	340
C	NOW GO THROUGH THE SAME PROCESS FOR CO2 + H2 = CO + H2O.	I	350
C		I	360
	CLOG2=(-1.98E-7)*TRIALT**2+(1.52E-3)*TRIALT-2.257	I	370
	KP2=10.**CLOG2	I	380
C		I	390
C	SUBROUTINE SECANT SOLVES FOR THE EQUILIBRIUM MOLAR FLOWRATES,	I	400
C	GIVEN A SET OF GOOD INITIAL GUESSES.	I	410
C		I	420
	X0(1)=FCO+1.E-10	I	430
	X0(2)=FCO2	I	440
	X0(3)=FH2+1.E-10	I	450
	X0(4)=FH2O	I	460
	X0(5)=F02+1.E-10	I	470
	N=5	I	480
	NDIGIT=5	I	490
	RNORM=0.	I	500
	CALL SECANT (X0,N,FCN,NDIGIT,RNORM)	I	510
	DO 102 JL=1,5	I	520
	IF (X0(JL).LT.0.) X0(JL)=1.E-10	I	530
102	CONTINUE	I	540
C		I	550
C	THE SOLUTIONS ARE STORED IN THE ARRAY X0. FIND THE NEW SPECIES	I	560
C	FLOWRATES IN LBMOL/HR.	I	570
		I	580

C	FFS02=FS02	I 590
	FFN2=FN2	I 600
	FFN0=FN0	I 610
	FFC0=X0(1)	I 620
	FFC02=X0(2)	I 630
	FFH2=X0(3)	I 640
	FFH20=X0(4)	I 650
	FF02=X0(5)	I 660
	FMLFLO=FFC0+FFC02+FFH2+FFH20+FFN0+FFN2+FF02+FFS02	I 670
C		I 680
C	FIND SPECIES MOLE FRACTIONS.	I 690
C		I 700
	XCO=FFC0/FMLFLO	I 710
	XC02=FFC02/FMLFLO	I 720
	XH2=FFH2/FMLFLO	I 730
	XH20=FFH20/FMLFLO	I 740
	XNO=FFN0/FMLFLO	I 750
	XN2=FFN2/FMLFLO	I 760
	XO2=FF02/FMLFLO	I 770
	XS02=FFS02/FMLFLO	I 780
	IF (RNORM.GT.-.5) GO TO 103	I 790
C		I 800
C	IF RNORM IS RETURNED NEGATIVE SUBROUTINE SECANT DID NOT CONVERGE.	I 810
C	TRY A DIFFERENT TEMPERATURE.	I 820
C		I 830
	IF (KOUNT.GE.4) GO TO 103	I 840
	WRITE (6,108) FFH20,FFC0,FFN2,FF02,FFC02,FFN0,FFS02,FFH2,TRIALT,XH	I 850
	120,XCO,XN2,XO2,XC02,XNO,XS02,XH2	I 860
	KOUNTP=KOUNT+1	I 870
	MK=KOUNT/2	I 880
	MKP=KOUNTP/2	I 890
	IF (MKP.GT.MK) TRIALT=TRIALT-500.	I 900
	IF (MKP.LE.MK) TRIALT=TRIALT+1000.	I 910
	GO TO 101	I 920
103	CONTINUE	I 930
	IF (IFLAG.EQ.1) GO TO 106	I 940
C		I 950
C	NOW SOLVE THE ENERGY EQUATION FOR TEMPERATURE AND SEE IF THE	I 960
C	INITIAL GUESS WAS ABOUT RIGHT.	I 970
C		I 980
	CALL TEMP (FFC0,FFC02,FFH2,FFH20,FFN0,FFN2,FF02,FFS02,TCHAR,FH,500	I 990
	1.,TRIALT,TOUT)	I 1000
C		I 1010
C	TEMP RETURNS THE TEMPERATURE CORRESPONDING TO THE EQUILIBRIUM	I 1020
C	MIXTURE. SEE IF IT AGREES WITH THE TRIAL TEMPERATURE.	I 1030
C		I 1040
	IF (ABS(TOUT-TRIALT).LE.2.) GO TO 104	I 1050
	TRIALT=TOUT	I 1060
	GO TO 101	I 1070
104	CONTINUE	I 1080
	WRITE (6,109) FFH20,FFC0,FFN2,FF02,FFC02,FFN0,FFS02,FFH2,TCHAR,TRI	I 1090
	1ALT	I 1100
C		I 1110
C	THE EQUILIBRIUM SOLUTION HAS CONVERGED. SEE IF THE KINETICALLY	I 1120
C	DETERMINED TEMPERATURE IS TOO HIGH.	I 1130
C		I 1140
	IF (T.GT.TRIALT) GO TO 105	I 1150
C		I 1160
C	SIMPLY RETURN IF NOT.	I 1170
C		I 1180

C	TOUT=T	I 1150
	JFLAG=0	I 1200
	RETURN	I 1210
C		I 1220
C	IF SO, REVERT TO EQUILIBRIUM VALUES SINCE KINETIC RESULTS ARE	I 1230
C	IN VIOLATION OF THE SECOND LAW.	I 1240
C		I 1250
105	CONTINUE	I 1260
	FCO=FFCO	I 1270
	FCO2=FFCO2	I 1280
	FFH2=FFH2	I 1290
	FFH2O=FFH2O	I 1300
	FFNO=FFNO	I 1310
	FFN2=FFN2	I 1320
	FFO2=FFO2	I 1330
	FFSO2=FFSO2	I 1340
	MOLFLO=FMLFLO	I 1350
	TOUT=TRIALT	I 1360
C		I 1370
C	SET JFLAG = 1 IF THE KINETIC RESULTS ARE IN VIOLATION.	I 1380
C		I 1390
C	JFLAG=1	I 1400
	RETURN	I 1410
106	CONTINUE	I 1420
	WRITE (6,109) FFH2O,FFCO,FFN2,FFO2,FFCO2,FFNO,FFSO2,FFH2,TCHAR,TRI	I 1430
	1ALT	I 1440
C		I 1450
C	CHECK THE CO2/CO RATIO FOR THE KINETIC AND EQUILIBRIUM CASES.	I 1460
C	IF THE KINETIC CASE IS HIGHER, SET JFLAG = 1 AND REVERT TO THE	I 1470
C	EQUILIBRIUM VALUES. OTHERWISE SET JFLAG = 0 AND RETURN.	I 1480
C		I 1490
	RAKIN=FCO2/FCO	I 1500
	RAEQU=FFCO2/FFCO	I 1510
	IF (RAKIN.GT.RAEQU.OR.FO2.LT.5.E-4) GO TO 105	I 1520
	JFLAG=0	I 1530
	RETURN	I 1540
107	CONTINUE	I 1550
	WRITE (6,110)	I 1560
	STOP	I 1570
C		I 1580
108	FORMAT (10X, 39HSUBROUTINE SECANT FAILED TO CONVERGE. , 54HGAS FL	I 1590
	10WRATES, TEMP, AND MOLE FRACTIONS ARE AS FOLLOW.,/,10X,8E10.3,10X,	I 1600
	2E10.3,/,10X,8E10.3,/,)	I 1610
109	FORMAT (1X, 8HEQLBRM ,10E10.3)	I 1620
110	FORMAT (/,10X, 39HSUBROUTINE EQLBRM WILL NOT CONVERGE.,/,)	I 1630
C		I 1640
	END	I 1650
	SUBROUTINE FCN (X,F,UDF)	I 1660
C		J 10
C	THIS SUBROUTINE CONTAINS THE SYSTEM OF NONLINEAR EQUATIONS.	J 20
C		J 30
	DIMENSION X(5), F(5)	J 40
	COMMON /E/ KP1,KP2,FFFCO,FFFCO2,FFFH2,FFFH2O,FFFN0,FFFN2,FFFO2,FFF	J 50
	1SO2	J 60
	REAL KP1,KP2	J 70
	UDF=0.	J 80
	F(1)=X(2)**2-(X(1)**2*X(5)/KP1**2)*(1./(X(1)+X(2)+X(3)+X(4)+X(5)+F	J 90
	1FFN2+FFFN0+FFFSO2))	J 100
	F(2)=X(4)-X(2)*X(3)*KP2/X(1)	J 110
		J 120

	F(3)=X(1)+X(2)-FFFCO-FFFCO2	J	130
	F(4)=X(3)+X(4)-FFFH2-FFFH2O	J	140
	F(5)=.5*(X(1)+X(4))+X(2)+X(5)-(.5*(FFFCO+FFFH2O)+FFFCO2+FFFO2)	J	150
	RETURN	J	160
C	END	J	170
	SUBROUTINE GASPAR (CHU,FLOCOL,EXAIR)	J	180
	COMMON /C/ FLOPRI,FLOSEC,TPRI,TSEC,ASH	K	10
	COMMON /F/ TRIALT,FFCO,FFCO2,FFH2,FFH2O,FFNO,FFN2,FFO2,FFSO2,FMLFL	K	20
10	REAL MMMG,MGY,N2,NO,MGHU	K	30
		K	40
C		K	50
C		K	60
C	CALCULATE PRODUCT GAS MOLE FRACTIONS.	K	70
		K	80
	CO=FFCO/FMLFLO	K	90
	CO2=FFCO2/FMLFLO	K	100
	H2=FFH2/FMLFLO	K	110
	H2O=FFH2O/FMLFLO	K	120
	NO=FFNO/FMLFLO	K	130
	N2=FFN2/FMLFLO	K	140
	O2=FFO2/FMLFLO	K	150
	SO2=FFSO2/FMLFLO	K	160
	MMMG=(CO+N2)*28.+CO2*44.+H2*2.+H2O*18.+NO*30.+O2*32.+SO2*64.	K	170
	MGY=FMLFLO*MMMG/FLOCOL	K	180
	CMF=(28.*CO+2.*H2)/MMMG	K	190
	CMGY=CMF*MGY	K	200
	MGHU=.00264*(H2*122970.+CO*121750.)	K	210
	RHO=.00264*MMMG	K	220
	CGEFF=MGHU*MGY/CHU/RHO	K	230
C		K	240
C	MMMG = MAKE GAS MOLECULAR WEIGHT, LB/LBMOLE.	K	250
C	MGY = MAKE GAS YIELD, LB MAKE GAS/LB COAL.	K	260
C	CMF = COMBUSTIBLE MASS FRACTION.	K	270
C	CMGY = COMBUSTIBLE MAKE GAS YIELD, LB COMB. GAS/LB COAL.	K	280
C	MGHU = MAKE GAS HEATING VALUE, BTU/SCF.	K	290
C	RHO = GAS DENSITY AT STP, LBMOLE/FT**3.	K	300
C	CGEFF = COLD GAS EFFICIENCY.	K	310
C	TO CALCULATE HOT GAS EFFICIENCY, FIND THE SENSIBLE ENTHALPY OF	K	320
C	THE PRODUCTS AND THE REACTANTS.	K	330
C		K	340
	TR=TPRI	K	350
	SHCOAL=HCOAL(TR)-HCOAL(537.)	K	360
	SHPA=FLOPRI/FLOCOL*(.233*(H02(TR)-H02(537.))+.767*(HN2(TR)-HN2(537	K	370
1.)))		K	380
	TR=TSEC	K	390
	SHSA=FLOSEC/FLOCOL*(.233*(H02(TR)-H02(537.))+.767*(HN2(TR)-HN2(537	K	400
1.)))		K	410
	SHREAC=SHPA+SHSA+SHCOAL	K	420
C		K	430
	TR=TRIALT	K	440
	SHPROD=FMLFLO/FLOCOL*(2.*H2*(HH2(TR)-HH2(537.))+18.*H2O*(HH2O(TR)-	K	450
	1HH2O(537.))+(28.*CO+30.*NO)*(HCO(TR)-HCO(537.))+(44.*CO2+64.*SO2)*	K	460
	2(HCO2(TR)-HCO2(537.))+28.*N2*(HN2(TR)-HN2(537.))+32.*O2*(H02(TR)-H	K	470
	3O2(537.)))	K	480
	HGEFF=CGEFF+(SHPROD-SHREAC)/CHU	K	490
	PCGEFF=100.*CGEFF	K	500
	PHGEFF=100.*HGEFF	K	510
	AIR=FLOPRI*FLOSEC	K	520
	WRITE (6,101) EXAIR,AIR,FLOCOL,TRIALT,MGY,CMGY,MGHU,PCGEFF,PHGEFF	K	530
	RETURN	K	540

C	101 FORMAT (////,10X, 18H**** GASIFICATION , 12HRESULTS ****,/,10X, 3	K	550
	10H((A/F)/(STOICHIOMETRIC A/F)), , 42HAIR AND COAL FEED RATES, FLAM	K	550
	2E TEMPERATURE,/,10X, 38HMAKE GAS YIELD, COMB. MAKE GAS YIELD, , 35	K	570
	3HHEATING VALUE,COLD GAS EFFICIENCY, AND , 33HHOT GAS EFFICIENCY AR	K	580
	4E AS FOLLOW.,/,10X,9E12.3,/,)	K	590
C	END	K	600
	FUNCTION HCOAL(T)	K	610
	HCOAL=.3*T	K	620
	RETURN	L	10
C	END	L	20
	FUNCTION HH2(T)	L	30
	HH2=(5.76*T+.000289*T**2+40.*T**.5)/2.	L	40
	RETURN	L	50
C	END	M	10
	FUNCTION HH20(T)	M	20
	HH20=(19.86*T-1194.*T**.5+7500.*ALOG(T))/18.	M	30
	RETURN	M	40
C	END	M	50
	FUNCTION HH20(T)	N	10
	HH20=(19.86*T-1194.*T**.5+7500.*ALOG(T))/18.	N	20
	RETURN	N	30
C	END	N	40
	FUNCTION HCO(T)	H	50
	HCO=(9.46*T-3290.*ALOG(T)-(1.07E6)/T)/28.	O	10
	RETURN	O	20
C	END	O	30
	FUNCTION HCO2(T)	O	40
	HCO2=(16.2*T-6530.*ALOG(T)-(1.41E6)/T)/44.	O	50
	RETURN	P	10
C	END	P	20
	FUNCTION HN2(T)	P	30
	HN2=(9.47*T-3470.*ALOG(T)-(1.16E6)/T)/28.	P	40
	RETURN	P	50
C	END	Q	10
	FUNCTION HQ2(T)	Q	20
	HQ2=(11.515*T-344.*T**.5+1530.*ALOG(T))/32.	Q	30
	RETURN	Q	40
C	END	Q	50
	FUNCTION HQ2(T)	R	10
	HQ2=(11.515*T-344.*T**.5+1530.*ALOG(T))/32.	R	20
	RETURN	R	30
C	END	R	40
	END	R	50

APPENDIX B. DATA REDUCTION PROGRAM

A. Program Structure

The data reduction program is divided into three main sections for analyzing data from methane combustion, coal combustion and coal gasification tests. A very brief introductory section establishes fixed constants and directs the user to the appropriate main section via logic statements. Most of the computing is performed within subroutines. The three main sections and the subroutines are described in this appendix; a listing of the program is also included.

B. Main Program

1. Methane Combustion

The three main program sections contain extensive input and output routines and single-use equations that are not amenable to subroutine format. Tables 12 and 13 list the input and output data for methane combustion trials. The ignition air and methane flowrates are measured with rotameters; they are calculated via a curve fit to the appropriate calibration. The methane calculation includes a correction factor for deviations in temperature and pressure from those that existed during the rotameter calibration (Brooks, 1963).

The equivalence ratio is defined as the experimental fuel/air ratio divided by the stoichiometric fuel/air ratio. The make gas molecular weight is found using the mole fractions provided by the mass spectrometer. Carbon to nitrogen and hydrogen to nitrogen ratios and the various mass balance errors serve as useful checks on the flow meters and mass spectrometer. The hydrogen and oxygen mass balance errors and the remainder of the output data are calculated in subroutines which will be detailed later in this appendix.

Table 12. Methane Combustion Input Variables

<u>Variable Description</u>	<u>Computer Name</u>	<u>Units</u>
barometric pressure	PBARO	in _{Hg}
sec. air temperature at reactor	SATR	°C
make gas temperature at reactor	MGTE	°C
ign. air temperature at reactor	IATR	°C
methane temperature at reactor	MTR	°C
sec. air temperature at meter	SATF	°C
make gas temperature at meter	MGTF	°C
sec. air gage pressure	SAGP	psig
sec. air orifice differential	SAPD	in _{Hg}
make gas gage pressure	MGGP	cm _{H₂O}
make gas orifice differential	MGPD	cm _{H₂O}
ign. air gage pressure	IAM	mm _{H₂O}
ign. air rotameter reading	IAR	cm
methane gage pressure	MM	mm _{H₂O}
methane rotameter reading	MR	cm
make gas mole fractions	H2, H2O, CO, CO2, N2, O2, CH4	

Table 13. Methane Combustion Output Variables

<u>Variable Description</u>	<u>Computer Name</u>	<u>Units</u>
corrected make gas temperature	TGAS	$^{\circ}\text{C}$
ignition air flowrate	IAFLO	lb/hr
methane flowrate	MFLO	lb/hr
secondary air flowrate	SAFLO	lb/hr
make gas flowrate	MGFLO	lb/hr
m.g. flowrate from subroutine AMGFLO	RMGFLO	lb/hr
make gas molecular weight	MMMG	lb/lbmole
equivalence ratio	ER	
percent heat loss	PERHL	%
input carbon/nitrogen ratio	ICN	
input hydrogen/nitrogen ratio	IHN	
exhaust carbon/nitrogen ratio	ECN	
exhaust hydrogen/nitrogen ratio	EHN	
carbon mass balance error	CMBE	%
hydrogen mass balance error	HMBE	%
oxygen mass balance error	OMBE	%
total mass balance error	TMBE	%
corrected product gas analyses	H ₂ , H ₂ O, CO, CO ₂ , N ₂ , O ₂ , CH ₄	

2. Coal Combustion

Tables 14 and 15 list the input and output data for coal combustion trials. Many of the data are the same as previously described in the methane combustion section. The coal feed rate is calculated from a curve fit to the feeder calibration. The air/coal input ratio and coal throughput are readily calculated from the total air flowrate and coal feed rate. The make gas yield, defined to be the ratio of the make gas flowrate to the coal feed rate, is also easily determined.

Carbon efficiency is a parameter of considerable interest in coal combustion and gasification and is discussed in detail in Chapters IV and V. Carbon efficiency is calculated via a carbon balance using the coal feed rate, fraction by weight of carbon in the coal, the make gas flowrate, and the make gas mole fractions of CO , CO_2 and CH_4 .

Parameters listed in Table 15 and not yet described are discussed with the appropriate subroutine description.

3. Coal Gasification

The reduction of data from coal gasification tests is somewhat more complicated than for methane or coal combustion. The input data for a coal gasification trial include those necessary for a combustion trial plus the steam temperature and pressure for flowrate and heat input calculations. The gasification output data include all the combustion data plus several performance indicators unique to gasification. Both the combustion and gasification parameters are summarized in Table 16.

The steam/coal input ratio and H_2/CO ratio are easily calculated from the mass flowrates and make gas mole fractions, respectively. The combustible mass fraction is also found from the product gas analysis:

$$\omega_p = (28 X_{\text{CO}} + 2 X_{\text{H}_2} + 16 X_{\text{CH}_4})/M \quad (\text{B-1})$$

where ω_p is the combustible mass fraction, X_i the mole fraction of species i and M the product gas molecular weight.

The combustible make gas yield is the product of the make gas yield and the combustible mass fraction and is expressed as

Table 14. Coal Combustion Input Variables

<u>Variable Description</u>	<u>Computer Name</u>	<u>Units</u>
barometric pressure	PBARO	in _{Hg}
pri. air temperature at reactor	PATF	°C
sec. air temperature at reactor	SATR	°C
make gas temperature at reactor	MGTE	°C
pri. air temperature at meter	PATFL	°C
sec. air temperature at meter	SATF	°C
make gas temperature at meter	MGTF	°C
pri. air gage pressure	PAGP	psig
pri. air orifice differential	PAPD	in _{H₂O}
sec. air gage pressure	SAGP	psig
sec. air orifice differential	SAPD	in _{Hg}
make gas gage pressure	MGGP	cm _{H₂O}
make gas orifice differential	MGPD	cm _{H₂O}
approx. ign. air flowrate	IAFLO	lb/hr
coal feeder speed	CFS	Hz
coal heating value	CHV	BTU/lb
coal mass fractions	CLC, CLO, CLH, CLN, CLS, CLASH, CLH2O	
make gas mole fractions	H2, H2O, CO, CO2, N2, O2, CH4	

Table 15. Coal Combustion Output Variables

<u>Variable Description</u>	<u>Computer Name</u>	<u>Units</u>
corrected make gas temperature	TGAS	$^{\circ}\text{C}$
ignition air flowrate	IAFLO	lb/hr
primary air flowrate	PAFLO	lb/hr
secondary air flowrate	SAFLO	lb/hr
coal feed rate	CFR	lb/hr
make gas flowrate	MGFLO	lb/hr
m.g. flowrate from subroutine	AMGFLO RMGFLO	lb/hr
make gas molecular weight	MMMG	lb/lbmole
equivalence ratio	ER	
carbon efficiency	CEFF	%
percent heat loss	PERHL	%
input hydrogen/nitrogen ratio	IHN	
exhaust hydrogen/nitrogen ratio	EHN	
air/coal input ratio	ACIR	
make gas yield	MGY	
coal throughput	CTHRU	lb/hrft ³
hydrogen mass balance error	HMBE	%
oxygen mass balance error	OMBE	%
total mass balance error	TMBE	%
corrected product gas analyses	H ₂ , H ₂ O, CO, CO ₂ , N ₂ , O ₂ , CH ₄	

Table 16. Coal Gasification Performance Indicators

<u>Parameter and Units</u>	<u>Computer Name</u>
air/coal input ratio, lbair/lbcoal	ACIR
steam/coal input ratio, lbsteam/lbcoal	SCIR
H ₂ /CO ratio	HCOR
percent heat loss, %	PERHL
carbon efficiency, %	CEFF
make gas yield, lbmake gas/lbcoal	MGY
coal throughput, lb/hrft ³	CTHRU
combustible make gas yield, lbcomb. gas/lbcoal	CMGY
combustible mass fraction	CMF
chemical yield, lbgas/lbcoal reacted	CY
steam decomposition, %	SD
make gas heating value, BTU/scf	MGHV
cold gas efficiency, %	CGEFF
hot gas efficiency, %	HGEFF

$$Y_p = Y \omega_p \quad (B-2)$$

where Y is the make gas yield. The chemical yield is defined to be the weight of gas produced per weight of coal reacted and is given by

$$\epsilon = Y / (1 - (1 - \eta_c) y_c) \quad (B-3)$$

where η_c is the carbon efficiency and y_c the coal carbon mass fraction.

Calculation of steam decomposition is complicated by the fact that some steam is produced from combustion of hydrogen released during pyrolysis. If it is assumed that all coal hydrogen is converted to steam, steam decomposition can be expressed as

$$SD = \frac{H_2O_{in} + (9y_H + y_{H_2O}) CFR - 18 X_{H_2O} \dot{m}_g / M}{H_2O_{in} + y_{H_2O} CFR} \quad (B-4)$$

where H_2O_{in} is the steam feed rate, y_H the coal hydrogen mass fraction, y_{H_2O} the coal moisture mass fraction, CFR the coal feed rate, X_{H_2O} the product gas H_2O mole fraction, $\dot{m}_g$ the gas flowrate and M the product gas molecular weight.

The make gas heating value is easily found from the gas analysis and the heats of combustion of the combustible constituents (Wark, 1971):

$$Q = \frac{1}{\rho_g} \sum X_i \Delta \bar{H}_{C,i} \quad (B-5)$$

where Q is the heating value (BTU/scf), ρ_g the gas density at STP (lbmole/ft³), X_i the mole fraction of species i and $\Delta \bar{H}_{C,i}$ the enthalpy of combustion of species i (BTU/lbmole).

Cold gas efficiency, a very important gasification parameter (George et al., 1977), is defined as the ratio of the product gas enthalpy of combustion (per weight of coal fed) to the coal enthalpy of combustion. Thus cold gas efficiency is that portion of the coal heating value present as chemical enthalpy in the product gas and is expressed as

$$\eta_{cg} = Q Y / \Delta H_{C,coal} \rho_g M \quad (B-6)$$

where $\Delta H_{C,coal}$ is the coal enthalpy of combustion (BTU/lb) and Q, Y, ρ_g and M are as previously defined.

Hot gas efficiency is a significant performance indicator when the sensible enthalpy of the product gas can be used directly. The hot gas efficiency 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)

$$\eta_{hg} = \eta_{cg} + \Delta H_{pr} / \Delta H_{C,coal} \quad (B-7)$$

where ΔH_{pr} is the difference in sensible enthalpy between reactants and products (BTU/lb coal).

C. Subroutines

1. Subroutine OFLO

The flowrate of any gas stream measured by an orifice meter is calculated by this subroutine. This includes primary and secondary air, steam and product gas flowrates. The equations used are adapted from ASME Power Test Codes (1959).

2. Subroutine AMGFL0

The exhaust gas orifice system proved unreliable due to water condensation and flyash accumulation. Subroutine AMGFL0 thus uses nitrogen gas as an inert tracer to independently calculate the exhaust gas flowrate. The nitrogen flowrate through the system is known from the input air flowrates, and the ratio of the nitrogen flowrate to that of each of the other exhaust gas constituents is known via the mass spectrometer analysis. Thus the total exhaust flowrate is calculated by summing the flowrates of the independent constituents. Note that since total mass is conserved in the reactor an independent check on the exhaust gas

flowrate is possible if the ash in the coal and any unreacted carbon are accounted for.

3. Subroutine COLFRM

In order to calculate the reactor heat loss in coal combustion and gasification tests, the coal enthalpy of formation must be known. The calculation of this quantity, performed in subroutine COLFRM, is best illustrated by example for the Rosebud seam coal of Table 17 (as received).

It is convenient at the outset to invent a molecule called CHONS that has the same molar ratios as the dry, ash-free coal:

$$\text{CHONS} = \text{CH}_{.777} \text{O}_{.153} \text{N}_{.012} \text{S}_{.006}$$

with $M = 15.6 \text{ lb/lbmole}$.

Stoichiometric combustion of one mole of CHONS is expressed as

The enthalpy of combustion of CHONS is calculated from the enthalpy of combustion of the parent coal as follows:

$$\Delta \bar{H}_{\text{C,CHONS}} = (-9900 \frac{\text{BTU}}{\text{lbcoal}}) (\frac{1 \text{ lbcoal}}{.7599 \text{ lbCHONS}}) (\frac{1 \text{ lbCHONS}}{15.6 \text{ lbmole}}) \quad (\text{B-9})$$

$$\Delta \bar{H}_{\text{C,CHONS}} = -203,240 \text{ BTU/lbmole}. \quad (\text{B-10})$$

The enthalpy of formation of CHONS can be found by rearranging the formula for enthalpy of combustion, generalized as follows (Wark, 1971):

$$\Delta \bar{H}_{\text{C}} = \sum_i (v_i \Delta \bar{H}_{f,i})_{\text{P}} - \sum_j (v_j \Delta \bar{H}_{f,j})_{\text{R}} \quad (\text{B-11})$$

where $\Delta \bar{H}_C$ is the enthalpy of combustion at 537R (BTU/lbmole), $\nu_{i,j}$ are stoichiometric coefficients for combustion of one mole of fuel, and the ΔH_f are enthalpies of formation at 537R (BTU/lbmole). Combining Eqns. (B-8) and (B-11) yields

$$\begin{aligned} \Delta \bar{H}_{C,CHONS} = & [(1)\Delta \bar{H}_{f,CO_2} + (.389)\Delta \bar{H}_{f,H_2O} + (.012)\Delta \bar{H}_{f,NO} + \\ & (.006)\Delta \bar{H}_{f,SO_2} + (4.25)\Delta \bar{H}_{f,N_2}] - [(1.13)\Delta \bar{H}_{f,O_2} + \\ & (4.25)\Delta \bar{H}_{f,N_2} + (1)\Delta \bar{H}_{f,CHONS}] \end{aligned} \quad (B-12)$$

Inserting values from Wark (1971) for enthalpies of formation and the CHONS enthalpy of combustion from Eqn. (B-10) yields

$$\Delta \bar{H}_{f,CHONS} = -14,200 \text{ BTU/lbmole} \quad (B-13)$$

The conversion to BTU/lbcoal finishes the example:

$$\Delta H_{f,coal} = \frac{(-14,200 \frac{\text{BTU}}{\text{lbmole}})(.7599 \frac{\text{lbCHONS}}{\text{lbcoal}})}{(15.6 \frac{\text{lbCHONS}}{\text{lbmole}})} \quad (B-14)$$

$$\Delta H_{f,coal} = -691 \text{ BTU/lb} \quad (B-15)$$

4. Subroutine CORECT

The exhaust gas temperature is measured by a thermocouple located as shown in Fig. 21. The thermocouple (T/C) temperature differs from the gas temperature due to radiation heat transfer; the object of subroutine CORECT is to calculate the gas temperature via a heat balance on the T/C bead. The basic assumptions and resulting heat balance are:

- (1) steady state
 - (2) negligible conduction heat transfer
- $$\begin{aligned} & (\text{rate of heat transfer to the T/C by convection}) - \\ & (\text{rate of heat transfer from the T/C by radiation}) = 0 \end{aligned} \quad (B-16)$$

Conduction losses are negligible because a significant length of T/C wire is exposed to the exhaust gases, preventing the formation of a temperature gradient in the vicinity of the T/C junction. Further assumptions and approximations will be made as necessary in the forthcoming analysis.

The first term of Eqn. (B-16) can be expressed by Newton's Law of Cooling (Holman, 1972)

$$\dot{Q}_c = hA_j(T_g - T) \quad (B-17)$$

where $\dot{Q}_c$ is the convection heat transfer (watts), h the heat transfer coefficient ($\text{w/m}^2\text{K}$), A_j the junction surface area (m^2), T_g the gas temperature ($^\circ\text{K}$) and T the junction temperature ($^\circ\text{K}$). The junction is roughly spherical and located at a point in the exhaust line where the gas velocity is very low (see Section V.B). Assuming a motionless fluid, the expression for Nusselt number for the junction is (Bird et al., 1960)

$$\text{Nu}_f = hD/k_g = 2.0 \quad (B-18)$$

where D is the sphere diameter (m) and k_g is the gas thermal conductivity ($\text{w/m}^\circ\text{K}$) evaluated at the mean of the gas and junction temperatures.

Pure gas thermal conductivities are tabulated by Vargaftik (1975) and Hilsenrath (1960). Curves have been fit to the tabulated data for computer calculations. The mixture thermal conductivity is calculated via Eqns. (B-19) and (B-20) (Bird et al., 1960):

$$k_g = \sum_i \frac{x_i k_i}{\sum_j x_j \phi_{ij}} \quad (B-19)$$

where

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2 \quad (B-20)$$

and X_i are mole fractions, k_g is thermal conductivity (w/mK), M molecular weight (g/gmole), and μ is viscosity (kg/ms). Tabulated data for pure gas viscosities have also been curve-fitted for computational purposes.

A very simple radiation heat transfer model is used to complete the heat balance. Radiation from the top and bottom sides of the junction are treated separately by passing a horizontal plane through the center of the junction. The following nomenclature is used:

$\dot{Q}_r \equiv$ net radiant heat transfer rate, w

$A_j \equiv$ junction surface area, m^2

$\dot{Q}_{TOP,BOT} \equiv$ net radiant heat transfer rate from the (top, bottom) of the junction, w

$A_{TOP,BOT} \equiv$ junction surface area (above, below) the mid-plane, m^2 ($A_{TOP} = A_{BOT} = \frac{1}{2}A_j$)

$T \equiv$ junction temperature, K

$T_c \equiv$ cooling coil surface temperature, K

$\epsilon_j \equiv$ junction emissivity

$\sigma \equiv$ Stefan-Boltzmann constant = $5.669 \times 10^{-8} \text{ w/m}^2\text{K}^4$

Shape factor calculations show that the top of the junction exchanges radiation almost exclusively with the cooling coil, and the bottom with the throat tube (see Fig. 12). Radiation from product gases can be neglected. The top of the junction is modeled as a convex object surrounded by the cooling coil via the following relation (Holman, 1972):

$$\dot{Q}_{TOP} = \sigma A_{TOP} \epsilon_j (T^4 - T_c^4) \quad (B-21)$$

By direct analogy, the heat transfer rate from the bottom of the junction is

$$\dot{Q}_{BOT} = \sigma A_{BOT} \epsilon_j (T^4 - T_T^4) \quad (B-22)$$

Combining Eqns. (B-21) and (B-22) yields

$$\dot{Q}_r = \sigma A_j \epsilon_j (T^4 - .5T_c^4 - .5T_T^4) \quad (B-23)$$

Values for ϵ_j , T_T and T_c are needed to find the heat transfer rate. The junction is often coated with soot and flyash, so a value of $\epsilon_j = .9$ is used (Chapman, 1974). The throat tube is heated very effectively by the swirling gases; a value of $T_T = T_g - 50$ is therefore used. The cooling coil is very cold compared to the junction temperature; moreover, the fourth power dependence of radiant heat transfer on temperature makes the coil temperature completely negligible. Thus a value of 0°K is chosen for computational ease.

The analysis is completed by inserting Eqns. (B-17) and (B-23) into the heat balance Eqn. (B-16):

$$h(T_g - T) - .9\sigma(T^4 - .5(T_g - 50)^4) = 0 \quad (B-24)$$

This expression is readily solved by Newton's method (Ketter and Prawel, 1969), converging after about four iterations. The gas temperature is typically 1200 to 1550 C during a test with corresponding junction temperatures of 1100 to 1370 C.

5. Subroutine HTLOSS

The heat loss from either reactor is defined to be any chemical or sensible enthalpy input that does not subsequently appear as chemical or sensible enthalpy in the product gas. The following formulas, adapted from Wark (1971), are used to calculate percent heat loss:

$$HL = (H_R - H_p) / \dot{Q}_{in} \quad (B-25)$$

$$H_R = \sum_i \dot{m}_i (\Delta H_f + h_{T_R} - h_{537})_i \quad (B-26)$$

$$H_p = \sum_j \dot{m}_j (\Delta H_f + h_{T_p} - h_{537})_j \quad (B-27)$$

$$\dot{Q}_{in} = \sum_i \dot{m}_i (\Delta H_c + h_{T_R} - h_{537})_i \quad (B-28)$$

where HL is heat loss (%), H_R total enthalpy of reactants (BTU/hr), H_p total enthalpy of products (BTU/hr), $\dot{Q}_{in}$ total energy input (BTU/hr), $\dot{m}$ mass flowrate (lb/hr), ΔH_c enthalpy of combustion at 537 R (BTU/lb), and $h_T - h_{537}$ the sensible enthalpy with reference to 537 R (BTU/lb).

The enthalpy of combustion of the coal is typically reported as the coal heating value (see Appendix C). The coal enthalpy of formation is calculated via subroutine COLFRM. All other necessary enthalpies of formation and combustion are tabulated in Wark (1971). The sensible enthalpies in Eqns. (B-26) through (B-28) are calculated by evaluating integrated specific heat formulas (Wark, 1971) for each species at the appropriate temperature. The specific heat of coal is not listed in Wark; a value of .3 BTU/lb $^{\circ}$ R is suggested by Smoot and Horton (1977). All the equations for sensible enthalpy are written as function subprograms for computational ease.

6. Subroutine BLNCE

This short subroutine determines the hydrogen and oxygen mass balance errors by comparing the flow of each species into and out of the reactor. For both species the mass balance error is expressed as

$$MBE = \frac{(\text{flow in} - \text{flow out})}{\text{flow in}}$$

Thus a positive error indicates a deficiency in the product gas.

7. Subroutine CRBERR

Carbon efficiency is perhaps the most important performance indicator for the cyclone reactor. An accurate product gas analysis is essential for reliable calculation of the carbon efficiency. Significant

hydrogen and oxygen mass balance errors cast doubt upon the validity of the gas analysis and thus the carbon efficiency. In subroutine CRBERR an error analysis is performed in which the impact of hydrogen and oxygen mass balance errors upon carbon efficiency are assessed.

The first step in the analysis is to add or subtract hydrogen and oxygen to the product gas stream so that the hydrogen and oxygen mass balance errors are zeroed. Since water vapor is a particularly difficult species to sample, the hydrogen surplus or deficiency is eliminated by changing the water vapor concentration. This method also changes the oxygen balance so a new oxygen mass balance error is calculated. This oxygen surplus or deficiency is then eliminated by dividing it among the O_2 , CO_2 and CO in the product gas in a manner that leaves their relative concentrations unaltered.

New mole fractions, product gas molecular weight and flowrate are then calculated. The solution is iterative because the original mass balance errors were calculated on the basis of an "erroneous" gas flowrate. Convergence is very rapid, and is followed by the calculation of a corrected carbon efficiency based on the new analysis. The typical change in carbon efficiency is about -5 percent.

8. Subroutine TOTERR

As mentioned in the description of subroutine AMGFLO, product gas flowrate is calculated by assuming a perfect N_2 balance across the reactor. Since total mass should also balance, a convenient check on the system is available and is carried out in subroutine TOTERR. The total reactant mass flowrate is compared to the exhaust gas flowrate plus the assumed exhaust flowrate of five unmeasured quantities: ash, unburned carbon, argon, NO and SO_2 . Typical total mass balance errors are 1 to 3 percent.

9. Subroutine DRY

Experience has shown that all product gas species except water vapor can be accurately measured by the mass spectrometer. Subroutine DRY generates an accurate product gas analysis by calculating mole

fractions on a dry basis and then determining the water vapor mole fraction via an oxygen balance.

The dry basis mole fractions are easily found by subtracting out the observed water vapor mole fraction and increasing the others proportionately. Water vapor is then added to the analysis in an amount that creates a perfect oxygen balance, and new mole fractions and a total gas flowrate are calculated. The analysis is usually self-consistent after only two iterations.

Since only the water vapor molar flowrate is changed in this analysis, carbon efficiency is unaltered. The virtue of this approach is demonstrated by the very low hydrogen mass balance errors that are achieved. Typical errors for methane and coal combustion are 3.4 and 8.9 percent, respectively.

D. Program Listing

	COMMON /A/ MCCCCG	A	10
	INTEGER DAY, YEAR, SA	A	20
	REAL IATR, MGTF, MGTE, MTR, MGGP, MGPD, IAM, IAR, MM, MR, MFLO, IAFLO, ICN, MU,	A	30
	1K, M	A	40
	REAL IHN, MMMG, N2, MGFLD, KMG, KPA, KSA, MGPD2, P, KS, MGY, MGHU	A	50
	DIMENSION X(7), MU(7), K(7), M(7)	A	60
C		A	70
C	THE LAST DATA CARD FOR A GIVEN DAY OR A GIVEN TYPE OF RUN MUST	A	80
C	BE A BLANK CARD. THREE BLANK CARDS MUST ALWAYS APPEAR AT THE	A	90
C	END OF ALL THE DATA TO TELL THE COMPUTER TO STOP.	A	100
C		A	110
	101 CONTINUE	A	120
	READ (5,122) FUEL1,FUEL2	A	130
C		A	140
C	PRINT THE NAME OF THE FUEL IN THE FIRST 20 SPACES OF THE	A	150
C	FIRST CARD.	A	160
C		A	170
	READ (5,123) MONTH, DAY, YEAR, MCCCCG, SA, NREACT, PBARD	A	180
	IF (MONTH.EQ.0) GO TO 121	A	190
C		A	200
C	MCCCCG=1 IF METHANE COMB, 2 IF COAL COMB, 3 IF COAL GASIFICATION	A	210
C	SA=1 IF LOW RANGE SECONDARY AIR, 2 IF HIGH RANGE SA	A	220
C	NREACT = 1 FOR CYCLONE REACTOR, 2 FOR JET.	A	230
C	PBARD = THE ATMOSPHERIC PRESSURE IN INCHES HG.	A	240
C		A	250
	DMG=.896	A	260
	KMG=.685	A	270
C		A	280
C	DMG = ORIFICE DIAMETER FOR MAKE GAS.	A	290
C	KMG = DISCHARGE COEFFICIENT FOR MAKE GAS.	A	300
C		A	310
	IF (SA.EQ.2) GO TO 102	A	320
C		A	330
C	LOW RANGE SA VALUES	A	340
C		A	350
	DSA=.113	A	360
	KSA=.575	A	370
C		A	380
C	DSA=ORIFICE DIAMETER FOR SA	A	390
C	KSA= DISCHARGE COEFFICIENT FOR SA	A	400
C		A	410
	GO TO 103	A	420
C		A	430
C	HIGH RANGE VALUES	A	440
C		A	450
	102 DSA=.209	A	460
	KSA=.596	A	470
	103 IF (MCCCCG-2) 104,109,115	A	480
C		A	490
C	METHANE COMBUSTION SECTION *****	A	500
C	THIS SECTION WAS WRITTEN FOR COMMERCIAL GRADE METHANE, WHOSE	A	510
C	EQUIVALENT CHEMICAL FORMULA IS C1.063H4.088 INSTEAD OF CH4. IF	A	520
C	SOME OTHER GRADE METHANE IS USED IN THE FUTURE THE PROGRAMMER	A	530
C	MUST ACCOUNT FOR CHANGES RESULTING FROM THE DIFFERENT FORMULA.	A	540
C		A	550
	104 READ (5,124) KOUNT, SATR, MGTF, SATF, MGTE, IATR, MTR	A	560
	IF (KOUNT.EQ.0) GO TO 101	A	570
C		A	580
C	KOUNT IS THE TRIAL NUMBER.	A	590
C		A	600

	READ (5,125) SAGP,SAPD,MGGP,MGPD,IAM,IAR,MM,MR	A 610
	READ (5,126) H2O,CH4,N2,O2,CO2,CO,H2	A 620
C		A 630
C	SATR= SECONDARY AIR TEMP AT REACTOR IN C	A 640
C	SATF=SEC AIR TEMP AT FLOWMETER IN C	A 650
C	MGTF=MAKE GAS(EXHAUST) TEMP AT FLOWMETER IN C	A 660
C	MGTE=MAKE GAS TEMP AT REACTOR EXIT IN C	A 670
C	IATR=IGNITION AIR TEMP AT ROTAMETER IN C	A 680
C	MTR=METHANE TEMP AT ROTAMETER IN C	A 690
C	SAGP=SECONDARY AIR GAGE PRESSURE IN PSI	A 700
C	SAPD=SECONDARY AIR PRESSURE DIFFERENTIAL IN INCHES OF MERCURY	A 710
C	MGGP=MAKE GAS GAGE PRESSURE IN CM OF WATER	A 720
C	MGPD=MAKE GAS PRESSURE DIFF IN CM OF WATER	A 730
C	IAM=IGNITION AIR MANOMETER READING IN MM OF WATER	A 740
C	IAR=IGNITION AIR ROTAMETER READING	A 750
C	MM=METHANE MANOMETER READING IN MM OF WATER	A 760
C	MR=METHANE ROTAMETER READING	A 770
C	CO,CO2,H2,H2O,N2,O2,CH4 ARE MOLE FRACTIONS IN PRODUCT GAS	A 780
C		A 790
	CLC=0.	A 800
	CLH2O=CLC	A 810
	CLO2=CLH2O	A 820
	CLH=CLO2	A 830
	CHF=0.	A 840
	CHU=CHF	A 850
	STFR=CHU	A 860
	PATF=STFR	A 870
	CFR=PATF	A 880
	SFLO=CFR	A 890
	PAFLO=SFLO	A 900
	WRITE (6,127) MONTH,DAY,YEAR,FUEL1,FUEL2	A 910
	WRITE (6,128) KOUNT	A 920
	WRITE (6,129) PBARO	A 930
	WRITE (6,130) IAM	A 940
	WRITE (6,131) IAR	A 950
	WRITE (6,132) IATR	A 960
	WRITE (6,133) MM	A 970
	WRITE (6,134) MR	A 980
	WRITE (6,135) MTR	A 990
	WRITE (6,136) SAGP	A 1000
	WRITE (6,137) SAPD	A 1010
	WRITE (6,138) SATF	A 1020
	WRITE (6,139) SATR	A 1030
	WRITE (6,140) MGGP	A 1040
	WRITE (6,141) MGPD	A 1050
	WRITE (6,142) MGTF	A 1060
	WRITE (6,143) MGTE	A 1070
	HWS=13.54*SAPD	A 1080
C		A 1090
C	HWS=SA PRESSURE DIFF IN INCHES OF WATER	A 1100
C		A 1110
	P=SAGP+.493*PBARO	A 1120
C		A 1130
C	P IS ABSOLUTE PRESSURE IN PSI	A 1140
C		A 1150
	RMW=29.	A 1160
C		A 1170
C	RMW IS THE MOLECULAR WEIGHT OF THE FLOWING MEDIUM.	A 1180
C		A 1190
	CALL OFLO (KSA,DSA,HWS,P,SATF,SAFLO,RMW)	A 1200

C		A 1210
C	SAFLO=SECONDARY AIR FLOWRATE IN LB/HR	A 1220
C		A 1230
C	IF (IAR.GT.9.5) GO TO 105	A 1240
	IAFLO=1.247*IAR*SQR((.0029*IAM+PBARO)/29.92)	A 1250
	GO TO 106	A 1260
105	IAFLO=SQR((.0029*IAM+PBARO)/29.92)*(-.033*IAR**2+1.683*IAR-1.32)	A 1270
106	IAFLO=IAFLO*.0639	A 1280
C		A 1290
C	IAFLO=IGNITION AIR FLOWRATE IN LB/HR	A 1300
C		A 1310
C	AIR=IAFLO+SAFLO	A 1320
	MFLO=3.636*MR*SQR(294.*(PBARO+.00291*MM)/29.92/(273.+MTR))/26.4	A 1330
C		A 1340
C	MFLO=METHANE FLOWRATE IN LB/HR	A 1350
C		A 1360
C	ER=17.30*MFLO/AIR	A 1370
C		A 1380
C	ER=EQUIVALENCE RATIO	A 1390
C		A 1400
C	ICN=1.147*MFLO/AIR	A 1410
C		A 1420
C	ICN=INPUT CARBON-NITROGEN RATIO	A 1430
C		A 1440
C	IHN=4.41*MFLO/AIR	A 1450
C		A 1460
C	IHN=INPUT HYDROGEN-NITROGEN RATIO	A 1470
C		A 1480
C	SUCH4=CH4	A 1490
	SUCO=CO	A 1500
	SUCU2=CU2	A 1510
	SUH2=H2	A 1520
	SUH2O=H2O	A 1530
	SUN2=N2	A 1540
	SUO2=O2	A 1550
	KCH=1	A 1560
	MMMG=28.*N2+16.*CH4+44.*CO2+18.*H2O+32.*O2+2.*H2+28.*CO	A 1570
C		A 1580
C	MMMG=MOLAR MASS OF MAKE GAS	A 1590
C	NOW USE THE ALTERNATE SCHEME FOR FINDING MAKE GAS FLOW RATE.	A 1600
C		A 1610
	CALL AMGFLO (AIR,H2,H2O,CO,CO2,N2,O2,CH4,RMGFLO)	A 1620
107	CONTINUE	A 1630
	MGP2=MGP2/2.54	A 1640
C		A 1650
C	MGP2= MGP2 IN INCHES WATER	A 1660
C		A 1670
C	P2=.493*PBARO+.0142*MGGP	A 1680
C		A 1690
C	P2= ABSOLUTE PRESSURE IN PSI	A 1700
C		A 1710
C	CALL OFLO (KMG,DMG,MGP2,P2,MGTF,MGFLO,MMMG)	A 1720
C		A 1730
C	MGFLO= MAKE GAS FLOWRATE IN LB/HR	A 1740
C	CORRECT THE MAKE GAS ORIFICE FLOW COEFFICIENT AND RECALCULATE.	A 1750
C		A 1760
	CKMG=(4.548E-7)*MGFLO**2-(2.026E-4)*MGFLO+.7035	A 1770
	CALL OFLO (CKMG,DMG,MGP2,P2,MGTF,MGFLO,MMMG)	A 1780
	ECN=.5*(CO2+CH4+CO)/N2	A 1790
C		A 1800

C	ECN=EXHAUST CARBON-NITROGEN RATIO	A 1810
C		A 1820
	$EHN=(H2O+2.*CH4)/N2$	A 1830
C		A 1840
C	EHN=EXHAUST HYDROGEN-NITROGEN RATIO	A 1850
C	CORRECT THE T/C READING FOR RADIATION.	A 1860
C		A 1870
	CALL CORECT (MGTE,MMMG,MU,RMGFLO,TGAS,X,K,M,H2,H2O,CO,CO2,N2,O2,CH	A 1880
	14)	A 1890
	$CMBE=100.*(ICN-ECN)/ICN$	A 1900
C		A 1910
C	CMBE = CARBON MASS BALANCE ERROR.	A 1920
C	CALCULATE REACTOR HEAT LOSS.	A 1930
C		A 1940
	CALL HTLOSS (PERHL,PAFLO,SAFLO,IAFLO,SFLO,CFR,MFLO,RMGFLO,CHU,H2,H	A 1950
	120,CO,CO2,N2,O2,CH4,MMMG,TGAS,SATR,PATF,MTR,IATR,STFR,CHF)	A 1960
	FMGFLO=AIR+MFLO	A 1970
C		A 1980
C	CALCULATE THE TOTAL MASS BALANCE ERROR.	A 1990
C		A 2000
	$TMBE=100.*(FMGFLO-RMGFLO)/FMGFLO$	A 2010
C		A 2020
C	PERFORM HYDROGEN AND OXYGEN MASS BALANCES.	A 2030
C		A 2040
	IF (KCH.EQ.1) CALL BLNCE (AIR,MFLO,CFR,SFLO,RMGFLO,CLH,CLO2,CLH2O,	A 2050
	1MMMG,H2,H2O,CO,CO2,O2,CH4,HMBE,OMBE)	A 2060
	WRITE (6,187) MONTH,DAY,YEAR,KOUNT	A 2070
	IF (KCH.EQ.1) WRITE (6,202)	A 2080
	IF (KCH.EQ.2) WRITE (6,203)	A 2090
	IF (KCH.EQ.3) WRITE (6,204)	A 2100
	WRITE (6,144) IAFLO	A 2110
	XIAFLO=IAFLO*15.65	A 2120
	WRITE (6,145) XIAFLO	A 2130
	WRITE (6,146) SAFLO	A 2140
	XSAFLO=SAFLO*15.65	A 2150
	WRITE (6,147) XSAFLO	A 2160
	WRITE (6,195) AIR	A 2170
	XAIR=AIR*15.65	A 2180
	WRITE (6,196) XAIR	A 2190
	WRITE (6,148) MFLO	A 2200
	XMF=MFLO*26.4	A 2210
	WRITE (6,149) XMF	A 2220
	WRITE (6,150) ER	A 2230
	WRITE (6,151) MGFLD	A 2240
	XMGFLO=MGFLO*454./MMMG	A 2250
	WRITE (6,152) XMGFLO	A 2260
	WRITE (6,153) RMGFLO	A 2270
	XRMG=RMGFLO*454./MMMG	A 2280
	WRITE (6,154) XRMG	A 2290
	WRITE (6,155) MMMG	A 2300
	WRITE (6,156) TGAS	A 2310
	WRITE (6,157) PERHL	A 2320
	WRITE (6,158) ICN	A 2330
	WRITE (6,159) IHN	A 2340
	WRITE (6,160) ECN	A 2350
	WRITE (6,161) EHN	A 2360
	WRITE (6,162) CMBE	A 2370
	IF (KCH.EQ.1) WRITE (6,215) HMBE,OMBE	A 2380
	IF (KCH.EQ.3) WRITE (6,216) HMBE	A 2390
	WRITE (6,163) TMBE	A 2400

	PCH4=100.*CH4	A 2410
	PCO=100.*CO	A 2420
	PCO2=100.*CO2	A 2430
	PH2=100.*H2	A 2440
	PH2O=100.*H2O	A 2450
	PN2=100.*N2	A 2460
	PO2=100.*O2	A 2470
	WRITE (6,218) PN2	A 2480
	WRITE (6,219) PO2	A 2490
	WRITE (6,220) PCO2	A 2500
	WRITE (6,221) PH2O	A 2510
	WRITE (6,222) PCO	A 2520
	WRITE (6,223) PCH4	A 2530
	WRITE (6,224) PH2	A 2540
	KCH=KCH+1	A 2550
	IF (KCH.GT.2) GO TO 108	A 2560
C		A 2570
C	GENERATE A NEW PRODUCT GAS ANALYSIS WITH SUBROUTINE CRBERR.	A 2580
C		A 2590
	CALL CRBERR (AIR,MFLO,SFLO,CFR,CLH,CLH2O,CLO2,CLC,RMGFLO,MMMG,N2,O	A 2600
	12,CO2,H2O,CO,H2,CH4,CCEFF,FMGFLO,FMMMG,FN2,F02,FCO2,FH2O,FCO,FH2,F	A 2610
	2CH4)	A 2620
	RMGFLO=FMGFLO	A 2630
	MMMG=FMMMG	A 2640
	N2=FN2	A 2650
	O2=F02	A 2660
	CO2=FCO2	A 2670
	H2O=FH2O	A 2680
	CO=FCO	A 2690
	H2=FH2	A 2700
	CH4=FCM4	A 2710
	GO TO 107	A 2720
108	CONTINUE	A 2730
	IF (KCH.GT.3) GO TO 104	A 2740
C		A 2750
C	GENERATE ANOTHER PRODUCT GAS ANALYSIS WITH SUBROUTINE DRY.	A 2760
C		A 2770
	CALL DRY (SUCCO,SUCCO2,SUHH2,SUHH2O,SUN2,SUO2,SUCH4,AIR,MFLO,SFLO,CFR,	A 2780
	1RMGFLO,MMMG,CLH,CLH2O,CLO2,CLC,CEFF,HMBE)	A 2790
	CO=SUCCO	A 2800
	CO2=SUCCO2	A 2810
	H2=SUHH2	A 2820
	H2O=SUHH2O	A 2830
	N2=SUN2	A 2840
	O2=SUO2	A 2850
	CH4=SUCH4	A 2860
	GO TO 107	A 2870
C		A 2880
C	COAL COMBUSTION SECTION *****	A 2890
C		A 2900
109	READ (5,166) CLC,CLO2,CLH,CLN,CLS,CLASH,CLH2O,CHU	A 2910
C		A 2920
C	CLC,CLO,CLH,CLN,CLS,CLASH ARE LB C,O,H,N,S,ASH PER LB COAL	A 2930
C	CHU= COAL HEATING VALUE IN BTU/LB	A 2940
C		A 2950
110	READ (5,164) KOUNT,PATFL,PATF,SATF,SATR,MGTF,MGTE	A 2960
	IF (KOUNT.EQ.0) GO TO 101	A 2970
	READ (5,165) PAGP,SAGP,MGGP,PAPD,SAPD,MGPD,IAFLO,CFS	A 2980
	READ (5,167) N2,O2,CO2,H2O,CO,CH4,H2	A 2990
C		A 3000

C	KOUNT IS THE TRIAL NUMBER.	A	3010
C	PATFL= PRIMARY AIR TEMP AT FLOWMETER IN C	A	3020
C	PATF= PRIMARY AIR TEMP AT FEEDER IN C	A	3030
C	SATF=SEC AIR TEMP AT FLOWMETER IN C	A	3040
C	SATR=SECONDARY AIR TEMP AT REACTOR IN C	A	3050
C	MGTF=MAKE GAS(EXHAUST) TEMP AT FLOWMETER IN C	A	3060
C	MGTE=MAKE GAS TEMP AT REACTOR EXIT IN C	A	3070
C	PAGP= PRIMARY AIR GAGE PRESSURE IN PSI	A	3080
C	SAGP=SECONDARY AIR GAGE PRESSURE IN PSI	A	3090
C	MGGP=MAKE GAS GAGE PRESSURE IN CM OF WATER	A	3100
C	PAPD= PRIMARY AIR PRESSURE DIFFERENTIAL IN INCHES WATER	A	3110
C	SAPD=SECONDARY AIR PRESSURE DIFFERENTIAL IN INCHES OF MERCURY	A	3120
C	MGPD=MAKE GAS PRESSURE DIFF IN CM OF WATER	A	3130
C	IAFLO= APPROXIMATE IGNITION AIR FLOWRATE IN LB/HR	A	3140
C	CFS = COAL FEEDER SPEED IN HZ.	A	3150
C	CO,CU2,H2,H2O,N2,O2,CH4 ARE PRODUCT GAS MOLE FRACTIONS.	A	3160
C		A	3170
	SFLO=0.	A	3180
	STFR=SFLO	A	3190
	MFLO=STFR	A	3200
	MTR=MFLO	A	3210
	IATR=30.	A	3220
	CFR=(-8.98E-5)*CFS**2+.15*CFS-1.28	A	3230
C		A	3240
C	CFR= COAL FEED RATE IN LB/HR	A	3250
C		A	3260
	WRITE (6,168) MONTH, DAY, YEAR, FUEL1, FUEL2	A	3270
	WRITE (6,169) KOUNT	A	3280
	WRITE (6,170) PBARO	A	3290
	WRITE (6,171) PAGP	A	3300
	WRITE (6,172) PAPD	A	3310
	WRITE (6,173) PATFL	A	3320
	WRITE (6,174) PATF	A	3330
	WRITE (6,175) SAGP	A	3340
	WRITE (6,176) SAPD	A	3350
	WRITE (6,177) SATF	A	3360
	WRITE (6,178) SATR	A	3370
	WRITE (6,179) MGGP	A	3380
	WRITE (6,180) MGPD	A	3390
	WRITE (6,181) MGTF	A	3400
	WRITE (6,182) MGTE	A	3410
	WRITE (6,183) CFR	A	3420
	WRITE (6,184) CHU	A	3430
	WRITE (6,185) IAFLO	A	3440
	PCLC=100.*CLC	A	3450
	PCL02=100.*CL02	A	3460
	PCLH=100.*CLH	A	3470
	PCLN=100.*CLN	A	3480
	PCLS=100.*CLS	A	3490
	PCLASH=100.*CLASH	A	3500
	PCLH20=100.*CLH20	A	3510
	WRITE (6,186) PCLC,PCL02,PCLH,PCLN,PCLS,PCLASH,PCLH20	A	3520
	HWS=13.54*SAPD	A	3530
C		A	3540
C	HWS=SA PRESSURE DIFF IN INCHES OF WATER	A	3550
C		A	3560
	P=SAGP+.493*PBARO	A	3570
C		A	3580
C	P IS ABSOLUTE PRESSURE IN PSI	A	3590
C		A	3600

	RMW=29.	A 3610
C		A 3620
C	RMW IS THE MOLECULAR WEIGHT OF THE FLOWING MEDIUM.	A 3630
C		A 3640
	CALL OFLO (KSA,DSA,HWS,P,SATF,SAFLO,RMW)	A 3650
	KPA=.561	A 3660
	DPA=.161	A 3670
	P=PACP+.493*FBARO	A 3680
	RMW=29.	A 3690
	CALL OFLO (KPA,DPA,PAPD,P,PATFL,PAFLO,RMW)	A 3700
C		A 3710
C	PAFLO= PRIMARY AIR FLOWRATE IN LB/HR	A 3720
C		A 3730
	AIR=PAFLO+SAFLO+IAFLO	A 3740
C		A 3750
C	AIR= TOTAL AIR FLOWRATE	A 3760
C		A 3770
	ACIR=AIR/CFR	A 3780
C		A 3790
C	ACIR= AIR/COAL INPUT RATIO	A 3800
C		A 3810
	AFS=34.32*(CLC/3.+CLH+CLS/8.-CLO2/8.)	A 3820
C		A 3830
C	AFS= AIR/FUEL STOICHIOMETRIC	A 3840
C		A 3850
	ER=AFS/ACIR	A 3860
C		A 3870
C	ER= EQUIVALENCE RATIO	A 3880
C		A 3890
	IHN=14.*CLH*CFR/(CLN*CFR+.768*AIR)	A 3900
C		A 3910
C	IHN= INPUT HYDROGEN/NITROGEN RATIO	A 3920
C		A 3930
	IF (NREACT.GT.1) GO TO 111	A 3940
	CTHRU=CFR/.176	A 3950
	GO TO 112	A 3960
111	CTHRU=CFR/5.285	A 3970
112	CONTINUE	A 3980
C		A 3990
C	CTHRU= COAL THROUGHPUT	A 4000
C		A 4010
	SUN2=N2	A 4020
	SUO2=O2	A 4030
	SUCO2=CO2	A 4040
	SUH2O=H2O	A 4050
	SUCO=CO	A 4060
	SUH2=H2	A 4070
	SUCH4=CH4	A 4080
C		A 4090
C	FIND COAL ENTHALPY OF FORMATION.	A 4100
C		A 4110
	CALL COLFRM (CLC,CLH,CLO2,CLN,CLS,CHU,CHF)	A 4120
	KCH=1	A 4130
	MMMG=28.*N2+32.*O2+18.*H2O+44.*CO2+28.*CO+16.*CH4+2.*H2	A 4140
C		A 4150
C	MMMG= MOLAR MASS MAKE GAS	A 4160
C	USE THE ALTERNATE METHOD TO CALCULATE MAKE GAS FLOWRATE.	A 4170
C		A 4180
	CALL AMGFLO (AIR,H2,H2O,CO,CO2,N2,O2,CH4,RMGFLO)	A 4190
	CEFF=12.*RMGFLO*(CO+CO2+CH4)/(MMMG*CFR*CLC)	A 4200

C		A 4210
C	CEFF= CARBON EFFICIENCY	A 4220
C		A 4230
113	CONTINUE	A 4240
	MGPD2=MGPD/2.54	A 4250
C		A 4260
C	MGPD2= MGPD IN INCHES WATER	A 4270
C		A 4280
	P2=.493*PBARO+.0142*MGCP	A 4290
C		A 4300
C	P2= ABSOLUTE PRESSURE IN PSI	A 4310
C		A 4320
	CALL OFLO (KMG,DMG,MGPD2,P2,MGTF,MGFLO,MMM)	A 4330
C		A 4340
C	MGFLO= MAKE GAS FLOWRATE IN LB/HR	A 4350
C	CORRECT THE MAKE GAS ORIFICE FLOW COEFFICIENT AND RECALCULATE.	A 4360
C		A 4370
	CKMG=(4.548E-7)*MGFLO**2-(2.026E-4)*MGFLO+.7035	A 4380
	CALL OFLO (CKMG,DMG,MGPD2,P2,MGTF,MGFLO,MMM)	A 4390
	MGY=RMGFLO/CFR	A 4400
C		A 4410
C	MGY= MAKE GAS YIELD	A 4420
C		A 4430
	EHN=(2.*H2O+4.*CH4)/(2.*N2)	A 4440
C		A 4450
C	EHN=EXHAUST HYDROGEN/NITROGEN RATIO	A 4460
C	CORRECT THE T/C READING FOR RADIATION.	A 4470
C		A 4480
	CALL CORECT (MGTE,MMM,MU,RMGFLO,TGAS,X,K,M,H2,H2O,CO,CO2,N2,O2,CH	A 4490
	14)	A 4500
C		A 4510
C	PERFORM HYDROGEN AND OXYGEN MASS BALANCES.	A 4520
C		A 4530
	IF (KCH.EQ.1) CALL BLNCE (AIR,MFLO,CFR,SFLO,RMGFLO,CLH,CLO2,CLH2O,	A 4540
	1MMM,H2,H2O,CO,CO2,O2,CH4,HMBE,OMBE)	A 4550
C		A 4560
C	CALCULATE THE TOTAL MASS BALANCE ERROR.	A 4570
C		A 4580
	CALL TOTERR (AIR,CFR,SFLO,RMGFLO,CLASH,CEFF,CLC,CLN,CLS,TMBE)	A 4590
C		A 4600
C	CALCULATE REACTOR HEAT LOSS.	A 4610
C		A 4620
	CALL HTLOSS (PERHL,PAFLO,SAFLO,IAFLO,SFLO,CFR,MFLO,RMGFLO,CHU,H2,H	A 4630
	120,CO,CO2,N2,O2,CH4,MMM,TGAS,SATR,PATF,MTR,IATR,STFR,CHF)	A 4640
	WRITE (6,187) MONTH,DAY,YEAR,KOUNT	A 4650
	WRITE (6,188)	A 4660
	WRITE (6,189) PAFLO	A 4670
	XPAFLO=PAFLO*15.65	A 4680
	WRITE (6,190) XPAFLO	A 4690
	WRITE (6,191) SAFLO	A 4700
	XSAFLO=SAFLO*15.65	A 4710
	WRITE (6,192) XSAFLO	A 4720
	WRITE (6,193) IAFLO	A 4730
	XIAFLO=IAFLO*15.65	A 4740
	WRITE (6,194) XIAFLO	A 4750
	WRITE (6,195) AIR	A 4760
	XAIR=AIR*15.65	A 4770
	WRITE (6,196) XAIR	A 4780
	WRITE (6,197) CFR	A 4790
	WRITE (6,198) ER	A 4800

WRITE (6,199) ACIR	A 4810
WRITE (6,200) CTHRU	A 4820
WRITE (6,201) IHN	A 4830
IF (KCH.EQ.1) WRITE (6,202)	A 4840
IF (KCH.EQ.2) WRITE (6,203)	A 4850
IF (KCH.EQ.3) WRITE (6,204)	A 4860
WRITE (6,205) MGFLO	A 4870
XMGFLO=MGFLO*454./MMMG	A 4880
WRITE (6,206) XMGFLO	A 4890
WRITE (6,207) RMGFLO	A 4900
XRMG=RMGFLO*454./MMMG	A 4910
WRITE (6,208) XRMG	A 4920
WRITE (6,209) MMMG	A 4930
WRITE (6,210) TGAS	A 4940
CEFF=100.*CEFF	A 4950
WRITE (6,211) CEFF	A 4960
WRITE (6,212) PERHL	A 4970
WRITE (6,213) EHN	A 4980
WRITE (6,214) MGY	A 4990
IF (KCH.EQ.1) WRITE (6,215) HMBE,OMBE	A 5000
IF (KCH.EQ.3) WRITE (6,216) HMBE	A 5010
WRITE (6,217) TMBE	A 5020
PCH4=100.*CH4	A 5030
PCO=100.*CO	A 5040
PCO2=100.*CO2	A 5050
PH2=100.*H2	A 5060
PH2O=100.*H2O	A 5070
PN2=100.*N2	A 5080
PO2=100.*O2	A 5090
WRITE (6,218) PN2	A 5100
WRITE (6,219) PO2	A 5110
WRITE (6,220) PCO2	A 5120
WRITE (6,221) PH2O	A 5130
WRITE (6,222) PCO	A 5140
WRITE (6,223) PCH4	A 5150
WRITE (6,224) PH2	A 5160
KCH=KCH+1	A 5170
IF (KCH.GT.2) GO TO 114	A 5180
C	A 5190
C	A 5200
C	H 5210
GENERATE A NEW PRODUCT GAS ANALYSIS WITH SUBROUTINE CRBERR.	A 5220
CALL CRBERR (AIR,MFLO,SFLO,CFR,CLH,CLH2O,CLO2,CLC,RMGFLO,MMMG,N2,O	A 5230
12,CO2,H2O,CO,H2,CH4,CCEFF,FMGFLO,FMMMG,PN2,F02,FCO2,FH2O,FCO,FH2,F	A 5240
2CH4)	A 5250
CEFF=CCEFF	A 5260
RMGFLO=FMGFLO	A 5270
MMMG=FMMMG	A 5280
N2=PN2	A 5290
O2=F02	A 5300
CO2=FCO2	A 5310
H2O=FH2O	A 5320
CO=FCO	A 5330
H2=FH2	A 5340
CH4=FCH4	A 5350
GO TO 113	A 5360
114 CONTINUE	A 5370
IF (KCH.GT.3) GO TO 110	A 5380
C	A 5390
C	A 5400
C	
GENERATE ANOTHER PRODUCT GAS ANALYSIS WITH SUBROUTINE DRY.	

	CALL DRY (SUCCO, SUCCO2, SUH2, SUH2O, SUN2, SUO2, SUCH4, AIR, MFLO, SFLO, CFR,	A 5410
	1RMGFLO, MMMG, CLH, CLH2O, CLO2, CLC, CEFF, HMBE)	A 5420
	CO=SUCCO	A 5430
	CO2=SUCCO2	A 5440
	H2=SUH2	A 5450
	H2O=SUH2O	A 5460
	N2=SUN2	A 5470
	O2=SUO2	A 5480
	CH4=SUCH4	A 5490
	GO TO 113	A 5500
C		A 5510
C	COAL GASIFICATION SECTION *****	A 5520
C		A 5530
	115 READ (5,225) CLC,CLO2,CLH,CLN,CLS,CLASH,CLH2O,CHU	A 5540
	116 READ (5,226) KOUNT,PATFL,PATF,SATF,SATR,MGTF,MGTE	A 5550
	IF (KOUNT.EQ.0) GO TO 101	A 5560
	READ (5,227) PACP,SAGP,MGGP,PAPD,SAPD,MGPD,IAFLO,CFS	A 5570
	READ (5,228) N2,O2,CO2,H2O,CO,CH4,H2	A 5580
	READ (5,229) SGP,SPD,STFL,STFR	A 5590
		A 5600
C	SGP= STEAM GAGE PRESSURE IN PSI	A 5610
C	SPD= STEAM PRESSURE DIFFERENTIAL IN INCHES WATER	A 5620
C	STFL= STEAM TEMP AT FLOWMETER IN C	A 5630
C	STFR= STEAM TEMP AT FEEDER/REACTOR IN C	A 5640
C	CFS = COAL FEEDER SPEED IN HZ.	A 5650
C		A 5660
	CFR=(-8.98E-5)*CFS**2+.15*CFS-1.28	A 5670
C		A 5680
C	CFR = COAL FEED RATE IN LB/HR.	A 5690
C		A 5700
	MFLO=0.	A 5710
	MTR=MFLO	A 5720
	IATR=30.	A 5730
	WRITE (6,230) MONTH,DAY,YEAR,FUEL1,FUEL2	A 5740
	WRITE (6,231) KOUNT	A 5750
	WRITE (6,232) PBARO	A 5760
	WRITE (6,233) PACP	A 5770
	WRITE (6,234) PAPD	A 5780
	WRITE (6,235) PATFL	A 5790
	WRITE (6,236) PATF	A 5800
	WRITE (6,237) SAGP	A 5810
	WRITE (6,238) SAPD	A 5820
	WRITE (6,239) SATF	A 5830
	WRITE (6,240) SATR	A 5840
	WRITE (6,241) MGGP	A 5850
	WRITE (6,242) MGPD	A 5860
	WRITE (6,243) MGTF	A 5870
	WRITE (6,244) MGTE	A 5880
	WRITE (6,245) SGP	A 5890
	WRITE (6,246) SPD	A 5900
	WRITE (6,247) STFL	A 5910
	WRITE (6,248) STFR	A 5920
	WRITE (6,249) CFR	A 5930
	WRITE (6,250) CHU	A 5940
	WRITE (6,251) IAFLO	A 5950
	PCLC=100.*CLC	A 5960
	PCLO2=100.*CLO2	A 5970
	PCLH=100.*CLH	A 5980
	PCLN=100.*CLN	A 5990
	PCLS=100.*CLS	A 6000

	PCLASH=100.*CLASH	A 6010
	PCLH2O=100.*CLH2O	A 6020
	WRITE (6,252) PCLC,PCL02,PCLH,PCLN,PCLS,PCLASH,PCLH2O	A 6030
	HWS=13.54*SAPD	A 6040
C		A 6050
C	HWS=SA PRESSURE DIFF IN INCHES OF WATER	A 6060
C		A 6070
	P=SAGP+.493*PBARO	A 6080
C		A 6090
C	P IS ABSOLUTE PRESSURE IN PSI	A 6100
C		A 6110
	RMW=29.	A 6120
C		A 6130
C	RMW IS THE MOLECULAR WEIGHT OF THE FLOWING MEDIUM.	A 6140
C		A 6150
	CALL OFLO (KSA,DSA,HWS,P,SATF,SAFLO,RMW)	A 6160
	KPA=.561	A 6170
	DPA=.161	A 6180
	P=PAGP+.493*PBARO	A 6190
	RMW=29.	A 6200
C		A 6210
C	RMW IS THE MOLECULAR WEIGHT OF THE FLOWING MEDIUM.	A 6220
C		A 6230
	CALL OFLO (KPA,DPA,PAPD,P,PATFL,PAFLO,RMW)	A 6240
C		A 6250
C	PAFLO= PRIMARY AIR FLOWRATE IN LB/HR	A 6260
C		A 6270
	AIR=PAFLO+SAFLO+IAFLO	A 6280
C		A 6290
C	AIR= TOTAL AIR FLOWRATE	A 6300
C		A 6310
	ACIR=AIR/CFR	A 6320
C		A 6330
C	ACIR= AIR/COAL INPUT RATIO	A 6340
		A 6350
	IF (NREACT.GT.1) GO TO 117	A 6360
	CTHRU=CFR/.176	A 6370
	GO TO 118	A 6380
	117 CTHRU=CFR/.5.PAS	A 6390
	118 CONTINUE	A 6400
C		A 6410
C	CTHRU= COAL THROUGHPUT	A 6420
C		A 6430
	KS=.56	A 6440
	DS=.17	A 6450
	P=.493*PBARO+SGP	A 6460
C		A 6470
C	P= ABSOLUTE PRESSURE IN PSI	A 6480
C		A 6490
	RMW=18.	A 6500
	CALL OFLO (KS,DS,SPD,P,STFL,SFLO,RMW)	A 6510
C		A 6520
C	SFLO= STEAM FLOWRATE IN LB/HR	A 6530
C		A 6540
	SCIR=SFLO/CFR	A 6550
C		A 6560
C	SCIR= STEAM/COAL INPUT RATIO	A 6570
C		A 6580
	AFS=34.32*(CLC/3.+CLH+CLS/8.-CLO2/8.)	A 6590
	ER=AFS/ACIR	A 6600

C		A 6610
C	ER = EQUIVALENCE RATIO BASED ON AIR FLOW.	A 6620
C		A 6630
	WRITE (6,265) MONTH, DAY, YEAR ,	A 6640
	WRITE (6,266) KOUNT	A 6650
	WRITE (6,188)	A 6660
	WRITE (6,253) PAFLO	A 6670
	XPAFLO=PAFLO*15.65	A 6680
	WRITE (6,254) XPAFLO	A 6690
	WRITE (6,255) SAFLO	A 6700
	XSAFLO=SAFLO*15.65	A 6710
	WRITE (6,256) XSAFLO	A 6720
	WRITE (6,257) IAFLO	A 6730
	XIAFLO=IAFLO*15.65	A 6740
	WRITE (6,258) XIAFLO	A 6750
	WRITE (6,195) AIR	A 6760
	XAIR=AIR*15.65	A 6770
	WRITE (6,196) XAIR	A 6780
	WRITE (6,259) SFLO	A 6790
	XSFL0=SFLO*25.2	A 6800
	WRITE (6,260) XSFL0	A 6810
	WRITE (6,261) CFR	A 6820
	WRITE (6,262) ACIR	A 6830
	WRITE (6,198) ER	A 6840
	WRITE (6,263) SCIR	A 6850
	WRITE (6,264) CTHRU	A 6860
	SUN2=N2	A 6870
	SUO2=O2	A 6880
	SUCO2=CO2	A 6890
	SUH2O=H2O	A 6900
	SUCO=CO	A 6910
	SUH2=H2	A 6920
	SUCH4=CH4	A 6930
C		A 6940
C	FIND COAL ENTHALPY OF FORMATION.	A 6950
C		A 6960
	CALL COLFRM (CLC,CLH,CLO2,CLN,CLS,CHU,CHF)	A 6970
	KCH=1	A 6980
	MMMG=28.*N2+32.*O2+18.*H2O+44.*CO2+28.*CO+16.*CH4+2.*H2	A 6990
C		A 7000
C	MMMG= MOLAR MASS MAKE GAS	A 7010
C	USE THE ALTERNATE METHOD TO CALCULATE MAKE GAS FLOWRATE.	A 7020
C		A 7030
	CALL AMGFLO (AIR,H2,H2O,CO,CO2,N2,O2,CH4,RMGFLO)	A 7040
	CEFF=12.*RMGFLO*(CO+CO2+CH4)/(MMMG*CFR*CLC)	A 7050
C		A 7060
C	CEFF= CARBON EFFICIENCY	A 7070
C		A 7080
	119 CONTINUE	A 7090
	MGPD2=MGPD/2.54	A 7100
C		A 7110
C	MGPD2= MGPD IN INCHES WATER	A 7120
C		A 7130
	P2=.493*PBARO+.0142*MGCP	A 7140
C		A 7150
C	P2= ABSOLUTE PRESSURE IN PSI	A 7160
C		A 7170
	CALL OFLO (KMG,DMG,MGPD2,P2,MGTF,MGFLO,MMMG)	A 7180
C		A 7190
C	MGFLO= MAKE GAS FLOWRATE IN LB/HR	A 7200

C	CORRECT THE MAKE GAS ORIFICE FLOW COEFFICIENT AND RECALCULATE.	A 7210
C		A 7220
	CKMG=(4.548E-7)*MGFLO**2-(2.026E-4)*MGFLO+.7035	A 7230
	CALL OFLO (CKMG, DMG, MGP'D2, P2, MGTf, MGFLO, MMMG)	A 7240
	MGY=RMGFLO/CFR	A 7250
C		A 7260
C	MGY= MAKE GAS YIELD	A 7270
C	CORRECT THE T/C READING FOR RADIATION.	A 7280
C		A 7290
	CALL CORECT (MGTE, MMMG, MU, RMGFLO, TGAS, X, K, M, H2, H2O, CO, CO2, N2, O2, CH	A 7300
	14)	A 7310
C		A 7320
C	PERFORM HYDROGEN AND OXYGEN MASS BALANCES.	A 7330
C		A 7340
	IF (KCH.EQ.1) CALL BLNCE (AIR, MFLO, CFR, SFLO, RMGFLO, CLH, CLH2O, CLH2O,	A 7350
	1MMMG, H2, H2O, CO, CO2, O2, CH4, HMBE, OMBE)	A 7360
C		A 7370
C	FIND THE TOTAL MASS BALANCE ERROR.	A 7380
C		A 7390
	CALL TOTERR (AIR, CFR, SFLO, RMGFLO, CLASH, CEFF, CLC, CLN, CLS, TMBE)	A 7400
C		A 7410
C	FIND THE REACTOR HEAT LOSS.	A 7420
C		A 7430
	CALL HTLOSS (PERHL, PAFLO, SAFLO, IAFLO, SFLO, CFR, MFLO, RMGFLO, CHU, H2, H	A 7440
	120, CO, CO2, N2, O2, CH4, MMMG, TGAS, SATR, PATF, MTR, IATR, STFR, CHF)	A 7450
	CMF=(28.*CO+2.*H2+16.*CH4)/MMMG	A 7460
C		A 7470
C	CMF= COMBUSTIBLE MASS FRACTION	A 7480
C		A 7490
	CMCY=CMF*MGY	A 7500
C		A 7510
C	CMGY=COMBUSTIBLE MAKE GAS YIELD	A 7520
C		A 7530
	CY=MGY/(1.-(1.-CEFF)*CLC)	A 7540
C		A 7550
C	CY= CHEMICAL YIELD	A 7560
C		A 7570
	HCOF=H2/CO	A 7580
C		A 7590
C	HCOF= H2/CO RATIO	A 7600
C		A 7610
	SD=(SFLO+CLH2O*CFR+9.*CLH*CFR-18.*H2O*RMGFLO/MMMG)/(SFLO+CLH2O*CFR	A 7620
	1)	A 7630
C		A 7640
C	SD=STEAM\DECOMPOSITION	A 7650
C		A 7660
	MGHV=.00264*(H2*122970.+CO*121750.+CH4*383040.)	A 7670
C		A 7680
C	MGHV = MAKE GAS HEATING VALUE IN BTU/SCUFT.	A 7690
C		A 7700
	RHO=.00264*MMMG	A 7710
	CGEFF=MGHV*MGY/CHU/RHO	A 7720
C		A 7730
C	CGEFF= COLD GAS EFFICIENCY	A 7740
C	HOT GAS EFFICIENCY CALCULATION.	A 7750
C	FIND THE SENSIBLE ENTHALPY OF EACH REACTANT.	A 7760
C	UNITS ARE BTU/LB COAL.	A 7770
C		A 7780
	TR=(PATF+273.)*1.8	A 7790
	SHCOAL=HCOAL(TR)-HCOAL(537.)	A 7800

	TR=(STFR+273.)*1.8	A 7810
	SHH2O=SFLO/CFR*(HH2O(TR)-HH2O(537.))	A 7820
	TR=(PATF+273.)*1.8	A 7830
	SHPA=PAFLO/CFR*(.233*(H02(TR)-H02(537.))+.767*(HN2(TR)-HN2(537.)))	A 7840
	TR=(SATR+273.)*1.8	A 7850
	SHSA=SAFLO/CFR*(.233*(H02(TR)-H02(537.))+.767*(HN2(TR)-HN2(537.)))	A 7860
	TR=(IATR+273.)*1.8	A 7870
	SHIA=IAFLO/CFR*(.233*(H02(TR)-H02(537.))+.767*(HN2(TR)-HN2(537.)))	A 7880
C		A 7890
C	NOW SUM TO FIND TOTAL SENSIBLE ENTHALPY.	A 7900
C		A 7910
	SHREAC=SHCOAL+SHH2O+SHPA+SHSA+SHIA	A 7920
C		A 7930
C	DO THE SAME FOR THE PRODUCT GASES.	A 7940
C		A 7950
	TR=(TGAS+273.)*1.8	A 7960
	SHPROD=RMGFLO/MMMG/CFR*(2.*H2*(HH2(TR)-HH2(537.))+19.*H2O*(HH2O(TR)-HH2O(537.))+28.*CO*(HCO(TR)-HCO(537.))+44.*CO2*(HCO2(TR)-HCO2(537.))+28.*N2*(HN2(TR)-HN2(537.))+32.*O2*(H02(TR)-H02(537.))+44.*CH4*3*(HCH4(TR)-HCH4(537.)))	A 7970
		A 7980
		A 7990
		A 8000
C		A 8010
C	NOW HOT GAS EFFICIENCY CAN BE COMPUTED.	A 8020
C		A 8030
	HGEFF=CGEFF+(SHPROD-SHREAC)/CHU	A 8040
	WRITE (6,265) MONTH, DAY, YEAR	A 8050
	WRITE (6,266) KOUNT	A 8060
	IF (KCH.EQ.1) WRITE (6,202)	A 8070
	IF (KCH.EQ.2) WRITE (6,203)	A 8080
	IF (KCH.EQ.3) WRITE (6,204)	A 8090
	WRITE (6,267) MGFL0	A 8100
	XMGFL0=MGFL0*454./MMMG	A 8110
	WRITE (6,268) XMGFL0	A 8120
	WRITE (6,269) RMGFL0	A 8130
	XRMG=RMGFL0*454./MMMG	A 8140
	WRITE (6,270) XRMG	A 8150
	WRITE (6,271) MMMG	A 8160
	WRITE (6,272) TGAS	A 8170
	CEFF=100.*CEFF	A 8180
	WRITE (6,273) CEFF	A 8190
	WRITE (6,274) PERHL	A 8200
	WRITE (6,275) MGHU	A 8210
	CGEFF=100.*CGEFF	A 8220
	WRITE (6,276) CGEFF	A 8230
	HGEFF=100.*HGEFF	A 8240
	WRITE (6,277) HGEFF	A 8250
	WRITE (6,278) MGY	A 8260
	WRITE (6,279) CMGY	A 8270
	WRITE (6,280) CMF	A 8280
	WRITE (6,281) CY	A 8290
	WRITE (6,282) HCOR	A 8300
	SD=100.*SD	A 8310
	WRITE (6,283) SD	A 8320
	IF (KCH.EQ.1) WRITE (6,215) HMBE,OMBE	A 8330
	IF (KCH.EQ.3) WRITE (6,216) HMBE	A 8340
	WRITE (6,284) TMBE	A 8350
	PCH4=100.*CH4	A 8360
	PCO=100.*CO	A 8370
	PCO2=100.*CO2	A 8380
	PH2=100.*H2	A 8390
	PH2O=100.*H2O	A 8400

	PN2=100.*N2	A 8410
	P02=100.*O2	A 8420
	WRITE (6,218) PN2	A 8430
	WRITE (6,219) P02	A 8440
	WRITE (6,220) PCO2	A 8450
	WRITE (6,221) PH2O	A 8460
	WRITE (6,222) PCO	A 8470
	WRITE (6,223) FCH4	A 8480
	WRITE (6,224) PH2	A 8490
	KCH=KCH+1	A 8500
	IF (KCH.GT.2) GO TO 120	A 8510
C		A 8520
C	GENERATE A NEW PRODUCT GAS ANALYSIS WITH SUBROUTINE CRBERR.	A 8530
C		A 8540
	CALL CRBERR (AIR,MFLO,SFLO,CFR,CLH,CLH2O,CLO2,CLC,RMGFLO,MMMG,N2,O	A 8550
	12,C02,H2O,CO,H2,CH4,CCEFF,FMGFLO,FMMMG,FN2,F02,FCO2,FH2O,FCO,FH2,F	A 8560
	2CH4)	A 8570
	CEFF=CCEFF	A 8580
	RMGFLO=FMGFLO	A 8590
	MMMG=FMMMG	A 8600
	N2=FN2	A 8610
	O2=F02	A 8620
	CO2=FCO2	A 8630
	H2O=FH2O	A 8640
	CO=FCO	A 8650
	H2=FH2	A 8660
	CH4=FCH4	A 8670
	GO TO 119	A 8680
120	CONTINUE	A 8690
	IF (KCH.GT.3) GO TO 116	A 8700
C		A 8710
C	GENERATE ANOTHER PRODUCT GAS ANALYSIS WITH SUBROUTINE DRY.	A 8720
C		A 8730
	CALL DRY (SU0,SUCO2,SUH2,SUH2O,SUN2,SUO2,SUCH4,AIR,MFLO,SFLO,CFR,	A 8740
	1RMGFLO,MMMG,CLH,CLH2O,CLO2,CLC,CEFF,HMBE)	A 8750
	CO=SUCO	A 8760
	CO2=SUCO2	A 8770
	H2=SUH2	A 8780
	H2O=SUH2O	A 8790
	N2=SUN2	A 8800
	O2=SUO2	A 8810
	CH4=SUCH4	A 8820
	GO TO 119	A 8830
121	CONTINUE	A 8840
	STOP	A 8850
C		A 8860
122	FORMAT (2A10)	A 8870
123	FORMAT (6I4,F10.0)	A 8880
124	FORMAT (I10,6F10.0)	A 8890
125	FORMAT (8F10.0)	A 8900
126	FORMAT (7F10.0)	A 8910
127	FORMAT (1H1,I2, 1H-,I2, 1H-,I2,5X,2A10,//)	A 8920
128	FORMAT (15H TRIAL NUMBER ,I3, 12H INPUT DATA,//)	A 8930
129	FORMAT (35H BAROMETRIC PRESSURE ,F7.2, 10H INCHES H	A 8940
	1G,//)	A 8950
130	FORMAT (35H IGNITION AIR MANOMETER ,F7.0, 12H MM OF WA	A 8960
	1TER,//)	A 8970
131	FORMAT (35H IGNITION AIR ROTAMETER ,F7.1,//)	A 8980
132	FORMAT (35H IGNITION AIR TEMP AT ROTAMETER ,F7.0, 10H DEGREES	A 8990
	1G,//)	A 9000

133	FORMAT (35H	METHANE MANOMETER	,F7.0, 12H MM OF WA	A 9010
	1TER, /)			A 9020
134	FORMAT (35H	METHANE ROTAMETER	,F7.1, /)	A 9030
135	FORMAT (35H	METHANE TEMP AT ROTAMETER	,F7.0, 10H DEGREES	A 9040
	1C, /)			A 9050
136	FORMAT (35H	SECONDARY AIR GAGE PRESSURE	,F7.0, 4H PSI, /)	A 9060
137	FORMAT (35H	SEC AIR PRESSURE DIFF	,F7.2, 10H INCHES H	A 9070
	1G, /)			A 9080
138	FORMAT (35H	SEC AIR TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A 9090
	1C, /)			A 9100
139	FORMAT (35H	SEC AIR TEMP AT REACTOR	,F7.0, 10H DEGREES	A 9110
	1C, /)			A 9120
140	FORMAT (35H	MAKE GAS GAGE PRESSURE	,F7.1, 9H CM WATER	A 9130
	1, /)			A 9140
141	FORMAT (35H	MAKE GAS PRESSURE DIFF	,F7.1, 9H CM WATER	A 9150
	1, /)			A 9160
142	FORMAT (35H	MAKE GAS TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A 9170
	1C, /)			A 9180
143	FORMAT (35H	MAKE GAS TEMP AT REACTOR EXIT	,F7.0, 10H DEGREES	A 9190
	1C, /)			A 9200
144	FORMAT (35H	IGNITION AIR FLOWRATE	,F7.1, 8H LB/HOUR)	A 9210
145	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9220
	1R)			A 9230
146	FORMAT (35H	SECONDARY AIR FLOWRATE	,F7.1, 6H LB/HR)	A 9240
147	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9250
	1R)			A 9260
148	FORMAT (35H	METHANE FLOWRATE	,F7.1, 6H LB/HR)	A 9270
149	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9280
	1R)			A 9290
150	FORMAT (35H	EQUIVALENCE RATIO	,F7.3, /)	A 9300
151	FORMAT (35H	MAKE GAS FLOWRATE	,F7.1, 6H LB/HR)	A 9310
152	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9320
	1R)			A 9330
153	FORMAT (35H	ALTERNATE MAKE GAS FLOWRATE	,F7.1, 6H LB/HR)	A 9340
154	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9350
	1R)			A 9360
155	FORMAT (35H	MAKE GAS MOLECULAR WEIGHT	,F7.1, 10H LB/LBMOL	A 9370
	1E, /)			A 9380
156	FORMAT (33H	CORRECTED MAKE GAS TEMPERATURE	,F7.0, 10H DEGREES C,	A 9390
	1 /)			A 9400
157	FORMAT (35H	PERCENT HEAT LOSS	,F7.1, 8H PERCENT,	A 9410
	1 /)			A 9420
158	FORMAT (35H	INPUT CARBON/NITROGEN RATIO	,F7.4, /)	A 9430
159	FORMAT (35H	INPUT HYDROGEN/NITROGEN RATIO	,F7.4, /)	A 9440
160	FORMAT (35H	EXHAUST CARBON/NITROGEN RATIO	,F7.4, /)	A 9450
161	FORMAT (35H	EXHAUST HYDROGEN/NITROGEN RATIO	,F7.4, /)	A 9460
162	FORMAT (35H	CARBON MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A 9470
	1 /)			A 9480
163	FORMAT (35H	TOTAL MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A 9490
	1 /)			A 9500
164	FORMAT (I10,6F10.0)			A 9510
165	FORMAT (8F10.0)			A 9520
166	FORMAT (8F10.0)			A 9530
167	FORMAT (7F10.0)			A 9540
168	FORMAT (1H1, I2, 1H-, I2, 1H-, I2, 5X, 2A10 /)			A 9550
169	FORMAT (15H	TRIAL NUMBER ,I3, 11H INPUT DATA, /)		A 9560
170	FORMAT (35H	BAROMETRIC PRESSURE	,F7.2, 10H INCHES H	A 9570
	1G, /)			A 9580
171	FORMAT (35H	PRIMARY AIR GAGE PRESSURE	,F7.0, 4H PSI, /)	A 9590
172	FORMAT (35H	PRIMARY AIR PRESSURE DIFF	,F7.2, 9H IN WATER	A 9600

173	FORMAT (35H	PRIMARY AIR TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A 9610
	1C, /)			A 9620
174	FORMAT (35H	PRIMARY AIR TEMP AT FEEDER	,F7.0, 10H DEGREES	A 9630
	1C, /)			A 9640
175	FORMAT (35H	SECONDARY AIR GAGE PRESSURE	,F7.0, 4H PSI, /)	A 9650
176	FORMAT (35H	SEC AIR PRESSURE DIFF	,F7.2, 10H INCHES H	A 9660
	1G, /)			A 9670
177	FORMAT (35H	SEC AIR TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A 9680
	1C, /)			A 9690
178	FORMAT (35H	SEC AIR TEMP AT REACTOR	,F7.0, 10H DEGREES	A 9700
	1C, /)			A 9710
179	FORMAT (35H	MAKE GAS GAGE PRESSURE	,F7.1, 9H CM WATER	A 9720
	1, /)			A 9730
180	FORMAT (35H	MAKE GAS PRESSURE DIFF	,F7.1, 9H CM WATER	A 9740
	1, /)			A 9750
181	FORMAT (35H	MAKE GAS TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A 9760
	1C, /)			A 9770
182	FORMAT (35H	MAKE GAS TEMP AT REACTOR EXIT	,F7.0, 10H DEGREES	A 9780
	1C, /)			A 9790
183	FORMAT (35H	COAL FEED RATE	,F7.2, 6H LB/HR, /)	A 9800
184	FORMAT (35H	COAL HEATING VALUE	,F7.0, 7H BTU/LB, /	A 9810
	1)			A 9820
185	FORMAT (35H	APPROX IGNITION AIR FLOWRATE	,F7.1, 6H LB/HR, /)	A 9830
186	FORMAT (19H	COAL WT PERCENT- ,F5.2, 2H C, F5.2, 2H O, F5.2, 2H		A 9840
	1H, F5.2, 2H N, F5.2, 3H S, F5.2, 4H ASH, F5.2, 4H H2O, /)			A 9850
187	FORMAT (1H1, I2, 1H-, I2, 1H-, I2, 18H	TRIAL NUMBER, I3, 7H		A 9860
	10OUTPUT, /)			A 9870
188	FORMAT (43H	DATA UNCHANGED BY THE CORRECTION ROUTINES, /)		A 9880
189	FORMAT (35H	PRIMARY AIR FLOWRATE	,F7.1, 6H LB/HR)	A 9890
190	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9900
	1R)			A 9910
191	FORMAT (35H	SECONDARY AIR FLOWRATE	,F7.1, 6H LB/HR)	A 9920
192	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9930
	1R)			A 9940
193	FORMAT (35H	IGNITION AIR FLOWRATE	,F7.1, 8H LB/HOUR)	A 9950
194	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9960
	1R)			A 9970
195	FORMAT (36H	TOTAL AIR FLOWRATE	,F7.1, 6H LB/HR)	A 9980
196	FORMAT (35H		,F7.1, 10H GMOLES/H	A 9990
	1R)			A10000
197	FORMAT (35H	COAL FEED RATE	,F7.2, 6H LB/HR, /)	A10010
198	FORMAT (35H	EQUIVALENCE RATIO	,F7.3, /)	A10020
199	FORMAT (35H	AIR/COAL INPUT RATIO	,F7.1, /)	A10030
200	FORMAT (35H	COAL THROUGHPUT	,F7.2, 9H LB/FT3HR	A10040
	1, /)			A10050
201	FORMAT (35H	INPUT H/N RATIO	,F7.4, /)	A10060
202	FORMAT (28H	RESULTS ACHIEVED WITH THE , 38HUNCORRECTED PRODUCT G		A10070
	1AS MOLE FRACTIONS, /)			A10080
203	FORMAT (31H	WHEN THE HYDROGEN AND OXYGEN , 38HMASS BALANCE ERROR		A10090
	1S ARE FORCED TO ZERO, /, 37H THE FOLLOWING RESULTS ARE ACHIEVED, /			A10100
	2)			A10110
204	FORMAT (35H	WHEN THE PRODUCT GAS IS ANALYZED , 14HON A DRY BASIS		A10120
	1, /, 32H AND H2O CONTENT IS CALCULATED , 21HUIA AN OXYGEN BALANCE,			A10130
	2/, 28H THE FOLLOWING RESULTS ARE , 9HACHIEVED, /)			A10140
205	FORMAT (35H	MAKE GAS FLOWRATE	,F7.1, 6H LB/HR)	A10150
206	FORMAT (35H		,F7.1, 10H GMOLES/H	A10160
	1R)			A10170
207	FORMAT (35H	ALTERNATE MAKE GAS FLOWRATE	,F7.1, 6H LB/HR)	A10180
208	FORMAT (35H		,F7.1, 10H GMOLES/H	A10190
				A10200

1R)			A10210
209	FORMAT (35H MAKE GAS MOLECULAR WEIGHT	,F7.1, 10H LB/LBMOL	A10220
1E, /)			A10230
210	FORMAT (33H CORRECTED MAKE GAS TEMPERATURE	,F7.0, 10H DEGREES C,	A10240
1 /)			A10250
211	FORMAT (35H CARBON EFFICIENCY	,F7.1, 8H PERCENT,	A10260
1 /)			A10270
212	FORMAT (35H PERCENT HEAT LOSS	,F7.1, 8H PERCENT,	A10280
1 /)			A10290
213	FORMAT (35H EXHAUST H/N RATIO	,F7.4, /)	A10300
214	FORMAT (35H MAKE GAS YIELD	,F7.1, 8H LBMG/CL,	A10310
1 /)			A10320
215	FORMAT (35H HYDROGEN MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A10330
1 /, 35H OXYGEN MASS BALANCE ERROR	,F7.2, 8H PERCENT, /)		A10340
216	FORMAT (35H HYDROGEN MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A10350
1 /)			A10360
217	FORMAT (35H TOTAL MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A10370
1 /)			A10380
218	FORMAT (35H MAKE GAS PERCENT N2	,F7.1, /)	A10390
219	FORMAT (35H MAKE GAS PERCENT O2	,F7.1, /)	A10400
220	FORMAT (35H MAKE GAS PERCENT CO2	,F7.1, /)	A10410
221	FORMAT (35H MAKE GAS PERCENT H2O	,F7.1, /)	A10420
222	FORMAT (35H MAKE GAS PERCENT CO	,F7.1, /)	A10430
223	FORMAT (35H MAKE GAS PERCENT CH4	,F7.1, /)	A10440
224	FORMAT (35H MAKE GAS PERCENT H2	,F7.1, /)	A10450
225	FORMAT (8F10.0)		A10460
226	FORMAT (I10.6F10.0)		A10470
227	FORMAT (8F10.0)		A10480
228	FORMAT (7F10.0)		A10490
229	FORMAT (4F10.0)		A10500
230	FORMAT (1H1, I2, 1H-, I2, 1H-, I2, 5X, 2A10, /)		A10510
231	FORMAT (15H TRIAL NUMBER , I3, 12H INPUT DATA, /)		A10520
232	FORMAT (35H BAROMETRIC PRESSURE	,F7.2, 10H INCHES H	A10530
1G, /)			A10540
233	FORMAT (35H PRIMARY AIR GAGE PRESSURE	,F7.0, 4H PSI, /)	A10550
234	FORMAT (35H PRIMARY AIR PRESSURE DIFF	,F7.2, 9H IN WATER	A10560
1, /)			A10570
235	FORMAT (35H PRIMARY AIR TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A10580
1C, /)			A10590
236	FORMAT (35H PRIMARY AIR TEMP AT FEEDER	,F7.0, 10H DEGREES	A10600
1C, /)			A10610
237	FORMAT (35H SECONDARY AIR GAGE PRESSURE	,F7.0, 4H PSI, /)	A10620
238	FORMAT (35H SEC AIR PRESSURE DIFF	,F7.2, 10H INCHES H	A10630
1G, /)			A10640
239	FORMAT (35H SEC AIR TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A10650
1C, /)			A10660
240	FORMAT (35H SEC AIR TEMP AT REACTOR	,F7.0, 10H DEGREES	A10670
1C, /)			A10680
241	FORMAT (35H MAKE GAS GAGE PRESSURE	,F7.1, 9H CM WATER	A10690
1, /)			A10700
242	FORMAT (35H MAKE GAS PRESSURE DIFF	,F7.1, 9H CM WATER	A10710
1, /)			A10720
243	FORMAT (35H MAKE GAS TEMP AT FLOWMETER	,F7.0, 10H DEGREES	A10730
1C, /)			A10740
244	FORMAT (35H MAKE GAS TEMP AT REACTOR EXIT	,F7.0, 10H DEGREES	A10750
1C, /)			A10760
245	FORMAT (35H STEAM GAUGE PRESSURE	,F7.0, 4H PSI, /)	A10770
246	FORMAT (35H STEAM PRESSURE DIFF	,F7.2, 7H IN H2O, /	A10780
1)			A10790
247	FORMAT (35H STEAM TEMP FLOWMETER	,F7.0, 10H DEGREES	A10800

1C, /)			A10810
248 FORMAT (35H	STEAM TEMP FEEDER/REACTOR	,F7.0, 10H DEGREES	A10820
1C, /)			A10830
249 FORMAT (35H	COAL FEED RATE	,F7.2, 6H LB/HR, /)	A10840
250 FORMAT (35H	COAL HEATING VALUE	,F7.0, 7H BTU/LB, /	A10850
1)			A10860
251 FORMAT (35H	APPROX IGNITION AIR FLOWRATE	,F7.1, 6H LB/HR, /)	A10870
252 FORMAT (19H	COAL WT PERCENT- ,F5.2, 2H C, F5.2, 2H O, F5.2, 2H		A10880
1H, F5.2, 2H N, F5.2, 3H S, F5.2, 4H ASH, F5.2, 4H H2O, /)			A10890
253 FORMAT (35H	PRIMARY AIR FLOWRATE	,F7.1, 6H LB/HR, /)	A10900
254 FORMAT (35H		,F7.1, 10H GMOLES/H	A10910
1R, /)			A10920
255 FORMAT (35H	SECONDARY AIR FLOWRATE	,F7.1, 6H LB/HR)	A10930
256 FORMAT (35H		,F7.1, 10H GMOLES/H	A10940
1R, /)			A10950
257 FORMAT (35H	IGNITION AIR FLOWRATE	,F7.1, 8H LB/HR)	A10960
258 FORMAT (35H		,F7.1, 10H GMOLES/H	A10970
1R, /)			A10980
259 FORMAT (35H	STEAM FLOWRATE	,F7.1, 6H LB/HR)	A10990
260 FORMAT (35H		,F7.1, 10H GMOLES/H	A11000
1R, /)			A11010
261 FORMAT (35H	COAL FEED RATE	,F7.2, 6H LB/HR, /)	A11020
262 FORMAT (35H	AIR/COAL INPUT RATIO	,F7.2, /)	A11030
263 FORMAT (35H	STEAM/COAL INPUT RATIO	,F7.3, /)	A11040
264 FORMAT (35H	COAL THROUGHPUT	,F7.2, 9H LB/FT3HR	A11050
1, /)			A11060
265 FORMAT (1H1, I2, 1H-, I2, 1H-, I2, /)			A11070
266 FORMAT (15H	TRIAL NUMBER ,I3, 8H OUTPUT, /)		A11080
267 FORMAT (35H	MAKE GAS FLOWRATE	,F7.1, 6H LB/HR)	A11090
268 FORMAT (35H		,F7.1, 10H GMOLES/H	A11100
1R, /)			A11110
269 FORMAT (35H	ALTERNATE MAKE GAS FLOWRATE	,F7.1, 6H LB/HR, /)	A11120
270 FORMAT (35H		,F7.1, 10H GMOLES/H	A11130
1R, /)			A11140
271 FORMAT (35H	MAKE GAS MOLECULAR WEIGHT	,F7.1, 10H LB/LBMOL	A11150
1E, /)			A11160
272 FORMAT (33H	CORRECTED MAKE GAS TEMPERATURE	,F7.0, 10H DEGREES C.	A11170
1/)			A11180
273 FORMAT (35H	CARBON EFFICIENCY	,F7.1, 8H PERCENT,	A11190
1/)			A11200
274 FORMAT (35H	PERCENT HEAT LOSS	,F7.1, 8H PERCENT,	A11210
1/)			A11220
275 FORMAT (35H	MAKE GAS HEATING VALUE	,F7.1, 8H BTU/SCF,	A11230
1/)			A11240
276 FORMAT (35H	COLD GAS EFFICIENCY	,F7.1, 8H PERCENT,	A11250
1/)			A11260
277 FORMAT (35H	HOT GAS EFFICIENCY	,F7.1, 8H PERCENT,	A11270
1/)			A11280
278 FORMAT (35H	MAKE GAS YIELD	,F7.1, 8H LBMG/CL,	A11290
1/)			A11300
279 FORMAT (35H	COMBUSTIBLE MAKE GAS YIELD	,F7.3, /)	A11310
280 FORMAT (35H	COMBUSTIBLE MASS FRACTION	,F7.3, /)	A11320
281 FORMAT (35H	CHEMICAL YIELD	,F7.1, 21H LBMG/LB	A11330
1COAL REACTED, /)			A11340
282 FORMAT (35H	H2/CO RATIO	,F7.3, /)	A11350
283 FORMAT (35H	STEAM DECOMPOSITION	,F7.1, 8H PERCENT,	A11360
1/)			A11370
284 FORMAT (35H	TOTAL MASS BALANCE ERROR	,F7.2, 8H PERCENT,	A11380
1/)			A11390
			A11400

C

	END	A11410
	SUBROUTINE DRY (CO,CO2,H2,H2O,N2,O2,CH4,AIR,MFLO,SFLO,CFR,RMGFLO,M	B 10
	1MMG,CLH,CLH2O,CLO2,CLC,CEFF,HMBE)	B 20
C		B 30
C	THIS SUBROUTINE CALCULATES THE PRODUCT GAS ANALYSIS ON A DRY	B 40
C	BASIS AND DETERMINES H2O VIA AN OXYGEN BALANCE.	B 50
		B 60
	COMMON /A/ MCCCCG	B 70
	REAL N2,MFLO,MMMG	B 80
C		B 90
C	CALCULATE MOLE FRACTIONS ON A DRY BASIS.	B 100
C		B 110
	D=1.-H2O	B 120
	DCO=CO/D	B 130
	DCO2=CO2/D	B 140
	DH2=H2/D	B 150
	DH2O=0.	B 160
	DN2=N2/D	B 170
	DO2=O2/D	B 180
	DCH4=CH4/D	B 190
	MMMG=28.*(DCO+DN2)+32.*DO2+44.*DCO2+2.*DH2+16.*DCH4	B 200
C		B 210
C	MMMG IS THE MAKE GAS MOLECULAR WEIGHT.	B 220
C	FIND THE MAKE GAS FLOWRATE.	B 230
C		B 240
	CALL AMGFLO (AIR,DH2,DH2O,DCO,DCO2,DN2,DO2,DCH4,RMGFLO)	B 250
C		B 260
C	FIND THE OXYGEN INPUT TO THE REACTOR, LBMOLE/HR.	B 270
C		B 280
	OIN=AIR*.42/28.84+SFLO/18.+CFR*(CLO2+16.*CLH2O/18.)/16.	B 290
C		B 300
C	FIND OXYGEN OUT IN LBMOLE/HR.	B 310
C		B 320
	101 OOUT=(RMGFLO/MMMG)*(2.*(DCO2+DO2)+DCO+DH2O)	B 330
C		B 340
C	OXYGEN ATOM DEFICIT IN PRODUCT GAS IN LBMOLE/HR.	B 350
C		B 360
	ODEF=OIN-OOUT	B 370
C		B 380
C	DEFICIT MOLE FRACTION IS AS FOLLOWS.	B 390
C		B 400
	OD=ODEF*MMMG/RMGFLO	B 410
	D=1.+OD	B 420
C		B 430
C	FIND NEW MOLE FRACTIONS.	B 440
		B 450
	FDN2=DN2/D	B 460
	FDO2=DO2/D	B 470
	FDCO2=DCO2/D	B 480
	FDCO=DCO/D	B 490
	FDCO2=DCO2/D	B 500
	FDCO2=DCO2/D	B 510
C		B 520
C	EACH MOLE OF OXYGEN ATOMS YIELDS ONE MOLE OF H2O ATOMS.	B 530
C		B 540
	DH2O=(DH2O+OD)/D	B 550
C		B 560
C	FIND NEW FLOWRATE.	B 570
C		B 580
	FMMMG=FDN2*28.+FDO2*32.+FDCO2*44.+FDH2O*18.+FDH2*2.+FDCO*28.+FDCO2*16.	B 590

	FMGFLO=FMMMG*RMGFLO*DN2/(MMMG*FDN2)	B	600
	MMMG=FMMMG	B	610
	RMGFLO=FMGFLO	B	620
	DN2=FDN2	B	630
C		B	640
C	CHECK FOR CONVERGENCE.	B	650
C		B	660
	IF (ABS(ODEF/DIN).LT..005) GO TO 102	B	670
	GO TO 101	B	680
102	CONTINUE	B	690
C		B	700
C	BYPASS THE CARBON EFFICIENCY CALCULATION FOR METHANE RUNS.	E	710
C		B	720
	IF (MCCCCG.LT.2) CEFF=1.	B	730
	IF (MCCCCG.LT.2) GO TO 103	B	740
	CEFF=12.*RMGFLO*(DCO+DCO2+DCH4)/(MMMG*CFR*CLC)	B	750
103	CONTINUE	B	760
C		B	770
C	CALCULATE HYDROGEN MASS BALANCE ERROR.	B	780
C		B	790
	HIN=MFLO*4.088/16.8+SFLO*2./18.+CFR*(CLH+CLH2O/9.)	B	800
	HOUT=(RMGFLO/MMMG)*2.*(DH2O+DH2+2.*DCH4)	B	810
	HMBE=100.*(HIN-HOUT)/HIN	B	820
	N2=DN2	B	830
	O2=DO2	B	840
	CO2=DCO2	B	850
	H2=DH2	B	860
	H2O=DH2O	B	870
	CO=DCO	B	880
	CH4=DCH4	B	890
	RETURN	B	900
C		B	910
	END	B	920
	SUBROUTINE CRBERR (AIR, MFLO, SFLO, CFR, CLH, CLH2O, CLO, CLC, RMGFLO, MMMG,	C	10
	1, N2, O2, CO2, H2O, CO, H2, CH4, CCEFF, FMGFLO, FMMMG, FN2, FO2, FCO2, FH2O, FCO,	C	20
	2FH2, FCH4)	C	30
	COMMON /A/ MCCCCG	C	40
	REAL MFLO, MMMG, N2	C	50
C		C	60
C	INITIALIZE THE PARAMETERS.	C	70
C	RESIDUAL OXYGEN IS DIVIDED AMONG CO, CO2, AND O2 ACCORDING TO	C	80
C	THEIR ORIGINAL MOLE FRACTIONS.	C	90
C		C	100
	TOTALO=CO2+O2+CO	C	110
	ADCO2=CO2/TOTALO	C	120
	ADO2=O2/TOTALO	C	130
	ADCO=CO/TOTALO	C	140
	FMMMG=MMMG	C	150
	FMGFLO=RMGFLO	C	160
	FN2=N2	C	170
	FO2=O2	C	180
	FCO2=CO2	C	190
	FH2O=H2O	C	200
	FCO=CO	C	210
	FH2=H2	C	220
	FCH4=CH4	C	230
C		C	240
C	FIND HYDROGEN AND OXYGEN ATOM FLOW RATES INTO AND OUT OF THE	C	250
C	REACTOR IN LBMOLES/HR.	C	260
C		C	270

	HIN=MFL0*4.088/16.8+SFL0*2./18.+CFR*(CLH+CLH20/9.)	C	280
	OIN=AIR*.42/28.84+SFL0/18.+CFR*(CLO+16.*CLH20/18.)/16.	C	290
101	HOUT=(FMGFLO/FMMMG)*(2.*FH20+2.*FH2+4.*FCH4)	C	300
	OOUT=(FMGFLO/FMMMG)*(2.*FCO2+2.*FO2+FCO+FH20)	C	310
C		C	320
C	THE WATER DEFICIT IN THE EXHAUST GAS IN LBMOL/HR IS AS FOLLOWS.	C	330
C		C	340
	H20DEF=(HIN-HOUT)/2.	C	350
C		C	360
C	THE OXYGEN DEFICIT IN LBMOL/HR IS AS FOLLOWS.	C	370
C		C	380
	O2DEF=(OIN-OOUT)/2.-H20DEF/2.	C	390
C		C	400
C	FIND DEFICIT MOLE FRACTIONS.	C	410
C		C	420
	H20D=H20DEF*FMMMG/FMGFLO	C	430
	O2D=O2DEF*FMMMG/FMGFLO	C	440
C		C	450
C	CORRECT THE PRODUCT GAS MOLE FRACTIONS.	C	460
C		C	470
	D=1.+H20D+O2D	C	480
	FN2=FN2/D	C	490
	FO2=(FO2+O2D*ADO2)/D	C	500
	FCO2=(FCO2+O2D*ADCO2)/D	C	510
	FCO=(FCO+O2D*ADCO)/D	C	520
	FH20=(FH20+H20D)/D	C	530
	FH2=FH2/D	C	540
	FCH4=FCH4/D	C	550
	FMMMG=FN2*28.+FO2*32.+FCO2*44.+FH20*18.+FCO*28.+FH2*2.+FCH4*16.	C	560
	FMGFLO=FMMMG*RMGFLO*N2/(MFMG*FN2)	C	570
C		C	580
C	IF BOTH DEFICITS ARE LESS THAN ONE PERCENT OF THE INPUT FLOW	C	590
C	THE ANALYSIS IS FINISHED.	C	600
C		C	610
	IF ((ABS(H20DEF/HIN).LT..01).AND.(ABS(O2DEF/OIN).LT..01)) GO TO 10	C	620
12		C	630
	GO TO 101	C	640
102	CONTINUE	C	650
C		C	660
C	BYPASS THE CARBON EFFICIENCY CALCULATION FOR METHANE RUNS.	C	670
C		C	680
	IF (MCCCCG.LT.2) CCEFF=1.	C	690
	IF (MCCCCG.LT.2) RETURN	C	700
C		C	710
C	CALCULATE THE CORRECTED CARBON EFFICIENCY.	C	720
C		C	730
	CCEFF=12.*FMGFLO*(FCO+FCO2+FCH4)/(FMMMG*CFR*CLC)	C	740
	RETURN	C	750
C		C	760
	END	C	770
	SUBROUTINE OFLO (K,D,HW,P,T,WH,RMW)	D	10
C		D	20
C	ORIFICE FLOWRATES SUBROUTINE	D	30
C		D	40
	REAL K	D	50
	Y=.692+.308*(P-.0364*HW)/P	D	60
	T2=(T+273.)*1.8	D	70
	GAMMA=144.*P*RMW/1545./T2	D	80
	WH=359.*K*D**2*Y*SQRT(HW*GAMMA)	D	90
C		D	100

C	WH = FLOWRATE IN LB/HR.	D	110
C		D	120
	RETURN	D	130
C		D	140
	END	D	150
	SUBROUTINE TOTERR (AIR,CFR,SFLO,RMGFLO,CLASH,CEFF,CLC,CLN,CLS,TMBE	E	10
	1)	E	20
C		E	30
C	CALCULATE THE TOTAL INPUT AND OUTPUT FLOWRATES, INCLUDING	E	40
C	COAL ASH, UNBURNT CARBON, ARGON, AND NO AND SO2.	E	50
C		E	60
	FIN=AIR+CFR+SFLO	E	70
	FOUT=RMGFLO+CLASH*CFR+(1.-CEFF)*CLC*CFR+.01286*AIR+(2.14*CLN+2.*CL	E	80
	15)*CFR	E	90
	TMBE=100.*(FIN-FOUT)/FIN	E	100
	RETURN	E	110
C		E	120
	END	E	130
	SUBROUTINE AMGFLO (AIR,H2,H2O,CO,CO2,N2,O2,CH4,RMGFLO)	F	10
	REAL N2	F	20
C		F	30
C	THIS IS AN ALTERNATE METHOD FOR FINDING THE MAKE GAS FLOWRATE.	F	40
C	FIND AIR FLOW IN GMOLES/HR.	F	50
C		F	60
	AIRGM=AIR*454./28.84	F	70
C		F	80
C	AIR IS 78.1 PERCENT NITROGEN.	F	90
C		F	100
	RN2=.781*AIRGM	F	110
C		F	120
C	RN2 IS THE TOTAL NITROGEN FLOW RATE IN GMOLES/HR. THE REST OF THE	F	130
C	PRODUCT GAS FLOWRATE CAN BE FOUND IN GMOLES / HR AS FOLLOWS.	F	140
C		F	150
	RO2=RN2*O2/N2	F	160
	RCO2=RN2*CO2/N2	F	170
	RH2O=RN2*H2O/N2	F	180
	RCO=RN2*CO/N2	F	190
	RCH4=RN2*CH4/N2	F	200
	RH2=RN2*H2/N2	F	210
C		F	220
C	NOW THE TOTAL MAKE GAS FLOWRATE IS FOUND BY SUMMING AND CONVERTING	F	230
C	TO LB/HR.	F	240
C		F	250
	RMGFLO=(32.*RO2+44.*RCO2+18.*RH2O+28.*(RCO+RN2)+16.*RCH4+2.*RH2)/4	F	260
	154.	F	270
	RETURN	F	280
C		F	290
	END	F	300
	SUBROUTINE HTLOSS (PERHL,PAFLO,SAFLO,IAFLO,SFLO,CFR,MFLO,RMGFLO,CH	G	10
	1U,H2,H2O,CO,CO2,N2,O2,CH4,MMMG,TGAS,SATR,PATF,MTR,IATR,STFR,CHF)	G	20
C		G	30
C	PERCENT HEAT LOSS SUBROUTINE	G	40
C		G	50
	REAL IAFLO,MFLO,N2,MMMG,IATR,MTR	G	60
C		G	70
C	FIRST THE TOTAL ENTHALPY OF THE REACTANTS IS CALCULATED AND	G	80
C	SUMMED UP. THCOAL = TOTAL ENTHALPY OF COAL.	G	90
C		G	100
	TR=(PATF+273.)*1.8	G	110
	THCOAL=CFR*(CHF+HCOAL(TR)-HCOAL(537.))	G	120

	SHCOAL=(HCOAL(TR)-HCOAL(537.))*CFR	G	130
	TR=(MTR+273.)*1.8	G	140
	THCH4=MFL0*(-2013.+HCH4(TR)-HCH4(537.))	G	150
	SHCH4=MFL0*(HCH4(TR)-HCH4(537.))	G	160
	TR=(STFR+273.)*1.8	G	170
	THH20=SFLO*(-5780.+HH20(TR)-HH20(537.))	G	180
	SHH20=SFLO*(HH20(TR)-HH20(537.))	G	190
C		G	200
C	NOTE THAT AIR IS 76.7 PERCENT N2 AND 23.3 PERCENT O2 BY WEIGHT.	G	210
C		G	220
	TR=(PATF+273.)*1.8	G	230
	THPA=(.233*(HO2(TR)-HO2(537.))+.767*(HN2(TR)-HN2(537.)))*PAFLO	G	240
	SHPA=THPA	G	250
	TR=(SATR+273.)*1.8	G	260
	THSA=(.233*(HO2(TR)-HO2(537.))+.767*(HN2(TR)-HN2(537.)))*SAFLO	G	270
	SHSA=THSA	G	280
	TR=(IATR+273.)*1.8	G	290
	THIA=(.233*(HO2(TR)-HO2(537.))+.767*(HN2(TR)-HN2(537.)))*IAFLO	G	300
	SHIA=THIA	G	310
C		G	320
C	NOW SUM UP TO FIND THE TOTAL.	G	330
C		G	340
	THREAC=THCOAL+THCH4+THH20+THPA+THSA+THIA	G	350
C		G	360
C	NOW DO THE SAME FOR THE PRODUCT GASES, WHICH ARE ALL AT THE SAME T	G	370
C		G	380
	TR=(TGAS+273.)*1.8	G	390
	THPROD=RMGFLO/MMMG*(2.*H2*(HH2(TR)-HH2(537.))+18.*H2O*(-5780.+HH2	G	400
	1(TR)-HH20(537.))+28.*CO*(-1698.+HCO(TR)-HCO(537.))+44.*CO2*(-3848.	G	410
	2+HCO2(TR)-HCO2(537.))+28.*N2*(HN2(TR)-HN2(537.))+32.*O2*(HO2(TR)-H	G	420
	3O2(537.))+16.*CH4*(-2013.+HCH4(TR)-HCH4(537.)))	G	430
C		G	440
C	DENOM = TOTAL CHEMICAL + SENSIBLE HEAT INPUT.	G	450
C		G	460
	DENOM=CHU*CFR+22758.*MFL0+SHCOAL+SHCH4+SHH20+SHPA+SHSA+SHIA	G	470
C		G	480
C	NOW CALCULATE PERCENT HEAT LOSS.	G	490
C		G	500
	PERHL=100.*(THREAC-THPROD)/DENOM	G	510
	RETURN	G	520
C		G	530
	END	G	540
C	FUNCTION SUBPROGRAMS TO BE USED WITH PERCENT HEAT LOSS SUBROUTINE.	H	10
C	UNITS ARE BTU/LBM.	H	20
C		H	30
	FUNCTION HH2(T)	H	40
	HH2=(5.76*T+.000289*T**2+40.*T**.5)/2.	H	50
	RETURN	H	60
C		H	70
	END	H	80
	FUNCTION HH20(T)	I	10
	HH20=(19.86*T-1194.*T**.5+7500.*ALOG(T))/18.	I	20
	RETURN	I	30
C		I	40
	END	I	50
	FUNCTION HCO(T)	J	10
	HCO=(9.46*T-3290.*ALOG(T)-(1.07E6)/T)/28.	J	20
	RETURN	J	30
C		J	40
	END	J	50

	FUNCTION HCO2(T)	K	10
	HCO2=(16.2*T-6530.*ALOG(T)-(1.41E6)/T)/44.	K	20
	RETURN	K	30
C		K	40
	END	K	50
	FUNCTION HN2(T)	L	10
	HN2=(9.47*T-3470.*ALOG(T)-(1.16E6)/T)/28.	L	20
	RETURN	L	30
C		L	40
	END	L	50
	FUNCTION HO2(T)	M	10
	HO2=(11.515*T-344.*T**.5+1530.*ALOG(T))/32.	M	20
	RETURN	M	30
C		M	40
	END	M	50
	FUNCTION HCH4(T)	N	10
	HCH4=(4.52*T+.003685*T**2)/16.	N	20
	RETURN	N	30
C		N	40
	END	N	50
	FUNCTION HCOAL(T)	O	10
	HCOAL=.3*T	O	20
	RETURN	O	30
C		O	40
	END	O	50
	SUBROUTINE CORECT (MGTE,MMMG,MU,RMGFLO,TGAS,X,K,M,H2,H2O,CO,CO2,N2	P	10
	1,O2,CH4)	P	20
C		P	30
C	THIS SUBROUTINE CORRECTS THE EXHAUST T/C READING FOR RADIATION.	P	40
C		P	50
	REAL MUH2,MUH2O,MUCO,MUCO2,MUN2,MUO2,MUCH4,MUMIX,KH2,KH2O,KCO,KCO2	P	60
	1,KN2,KO2,KCH4,KMIX,MGTE,MMMG,MU,K,M,N2,MGTE2	P	70
	DIMENSION X(7), MU(7), K(7), M(7)	P	80
	KOUNT=0	P	90
	TPR=MGTE+273.	P	100
101	TPRCP=TPR*1.8	P	110
C		P	120
C	TPR IS THE TEMPERATURE AT WHICH CONDUCTIVITY AND VISCOSITY ARE	P	130
C	EVALUATED IN DEG K. TPRCP = TPR IN DEG R FOR CP CALCULATIONS.	P	140
C	K VALUES ARE IN W/M K.	P	150
C		P	160
	KH2=(4.525E-4)*TPR-.027	P	170
	KH2O=(1.345E-4)*TPR-.0367	P	180
	KCO=(5.225E-5)*TPR+.0141	P	190
	KCO2=(6.E-5)*TFR+.0081	P	200
	KN2=(5.575E-5)*TPR+.00895	P	210
	KO2=(5.325E-5)*TPR+.01775	P	220
	KCH4=(1.86E-4)*TPR-.026	P	230
C		P	240
C	MU VALUES ARE IN KG/M S.	P	250
C		P	260
	MUH2=(-2.854E-12)*TPR**2+(1.93E-8)*TPR+3.607E-6	P	270
	MUH2O=(-1.825E-11)*TPR**2+(7.75E-8)*TPR-2.345E-5	P	280
	MUCO=(-4.75E-12)*TPR**2+(3.735E-8)*TPR+9.093E-6	P	290
	MUCO2=(-2.46E-12)*TPR**2+(2.84E-8)*TPR+1.441E-5	P	300
	MUN2=(-2.406E-12)*TPR**2+(2.615E-8)*TPR+1.682E-5	P	310
	MUO2=(-3.387E-12)*TPR**2+(3.341E-8)*TPR+1.82E-5	P	320
	MUCH4=(-1.328E-11)*TPR**2+(3.631E-8)*TPR+8.8E-7	P	330
C		P	340
C	CP VALUES ARE IN W S/KGMOLE K.	P	350

C	CPH2=24115.+2.42*TPRCP+83734./SQRT(TPRCP)	P 360
	CPH20=83148.-(2.499E6)/SQRT(TPRCP)+(3.14E7)/TPRCP	P 370
	CPC0=39606.-(1.377E7)/TPRCP+(4.48E9)/TPRCP**2	P 380
	CPC02=67824.-(2.734E7)/TPRCP+(5.903E9)/TPRCP**2	P 390
	CPN2=39648.-(1.453E7)/TPRCP+(4.857E9)/TPRCP**2	P 400
	CP02=48210.-(7.201E5)/SQRT(TPRCP)+(6.406E5)/TPRCP	P 410
	CPCH4=18924.+30.86*TPRCP	P 420
	K(1)=KH2	P 430
	K(2)=KH20	P 440
	K(3)=KCO	P 450
	K(4)=KCO2	P 460
	K(5)=KN2	P 470
	K(6)=KO2	P 480
	K(7)=KCH4	P 490
	MU(1)=MUH2	P 500
	MU(2)=MUH20	P 510
	MU(3)=MUCO	P 520
	MU(4)=MUCO2	P 530
	MU(5)=MUN2	P 540
	MU(6)=MUO2	P 550
	MU(7)=MUCH4	P 560
	X(1)=H2	P 570
	X(2)=H20	P 580
	X(3)=CO	P 590
	X(4)=CO2	P 600
	X(5)=N2	P 610
	X(6)=O2	P 620
	X(7)=CH4	P 630
	M(1)=2.	P 640
	M(2)=18.	P 650
	M(3)=28.	P 660
	M(4)=44.	P 670
	M(5)=28.	P 680
	M(6)=32.	P 690
	M(7)=16.	P 700
C		P 710
C	NOW MU AND K FOR THE MIXTURE CAN BE CALCULATED.	P 720
C		P 730
	SUMMU=0.	P 740
	SUMK=0.	P 750
	DO 103 I=1,7	P 760
	SUM2=0.	P 770
	DO 102 J=1,7	P 780
	SUM2=SUM2+X(J)*((1.+SQRT(MU(I)/MU(J)))*(M(J)/M(I))**.25)**2/SQ	P 790
	RT(8.*(1.+M(I)/M(J)))	P 800
1	CONTINUE	P 810
102	SUMMU=SUMMU+X(I)*MU(I)/SUM2	P 820
	SUMK=SUMK+X(I)*K(I)/SUM2	P 830
103	CONTINUE	P 840
	MUMIX=SUMMU	P 850
	KMIX=SUMK	P 860
C		P 870
C	NOW FIND CP OF THE MIXTURE.	P 880
C	UNITS ARE W S/KG K.	P 890
C		P 900
	CPMIX=(H2*CPH2+H20*CPH20+CO*CPC0+CO2*CPC02+N2*CPN2+O2*CP02+CH4*CPC	P 910
	1H4)/MMMG	P 920
C		P 930
C	NOW PRANDTL AND REYNOLDS NUMBERS ARE FOUND.	P 940
		P 950

C	PR=MUMIX*CPMIX/KMIX	P 960
	RE=.000258*RMGFLO/MUMIX	P 970
C		P 980
C	THE T/C BEAD IS LOCATED IN A WEAK RECIRCULATION ZONE.	P 990
C	USE THE NUSSELT NUMBER FOR THE STATIC CASE = 2.	P 1000
C	THE PRANDTL AND REYNOLDS NUMBER CALCULATIONS HAVE BEEN LEFT	P 1010
C	INTACT IN CASE SOME OTHER NUSSELT NUMBER CORRELATION IS	P 1020
C	ADOPTED IN THE FUTURE.	P 1030
C		P 1040
C	H=2.*KMIX/.003175	P 1050
C		P 1060
C	NOW THE T/C HEAT BALANCE CAN BE USED TO FIND T _{GAS} BY AN	P 1070
C	ITERATIVE PROCESS.	P 1080
C		P 1090
C	EPS=.9	P 1100
	SIGMA=5.6697E-9	P 1110
C		P 1120
C	NEWTON'S METHOD WILL BE USED TO FIND THE GAS TEMPERATURE. THE	P 1130
C	T/C TEMPERATURE WILL BE USED AS A FIRST GUESS. UNITS ARE DEG K.	P 1140
C		P 1150
	MGTE2=MGTE+273.	P 1160
	TGAS1=MGTE2	P 1170
104	F=H*(TGAS1-MGTE2)+EPS*SIGMA*(.5*(TGAS1-50.))**4-MGTE2**4)	P 1180
	DFDT=H+EPS*SIGMA*(2.*(TGAS1-50.))**3)	P 1190
	TGAS2=TGAS1-F/DFDT	P 1200
	IF ((TGAS2-TGAS1).LT.1.) GO TO 105	P 1210
	TGAS1=TGAS2	P 1220
	GO TO 104	P 1230
105	CONTINUE	P 1240
	IF (KOUNT.EQ.1) GO TO 106	P 1250
	KOUNT=1	P 1260
C		P 1270
C	ITERATE ONCE WITH A CORRECTED GAS TEMPERATURE.	P 1280
C		P 1290
	TPR=(TPR+TGAS2)/2.	P 1300
	GO TO 101	P 1310
106	TGAS=TGAS2-273.	P 1320
C		P 1330
C	RETURN T _{GAS} IN DEG C.	P 1340
C		P 1350
C	RETURN	P 1360
C		P 1370
	END	P 1380
	SUBROUTINE COLFRM (CLC,CLH,CLO,CLN,CLS,CHV,CHF)	P 1390
	REAL M	Q 10
C		Q 20
C	DERIVE CHONS FORMULA FOR ASH- AND MOISTURE-FREE COAL.	Q 30
C		Q 40
	A=12.*CLH/CLC	Q 50
	B=(12./16.)*CLO/CLC	Q 60
	C=(12./14.)*CLN/CLC	Q 70
	D=(12./32.)*CLS/CLC	Q 80
C		Q 90
C	FIND MOLECULAR WEIGHT OF CHONS.	Q 100
C		Q 110
	M=12.+A*B*16.+C*14.+D*32.	Q 120
C		Q 130
C	FIND HEAT OF COMBUSTION OF CHONS.	Q 140
C		Q 150
C	UNITS ARE BTU/LBMOLE CHONS.	Q 160

C	DELTHC=-CHU*M/(CLC+CLH+CLO+CLN+CLS)	Q	170
C		Q	180
C	NOW FIND THE HEAT OF FORMATION OF CHONS IN BTU/LBMOLE CHONS.	Q	190
C		Q	200
C	CHONSF=-169290.+.5*A*(-122970.)+L*38880.+D*(-127700.)-DELTHC	Q	210
C		Q	220
C	CONVERT TO BTU/LB COAL.	Q	230
C		Q	240
C	CHF=CHONSF*(CLC+CLH+CLO+CLN+CLS)/M	Q	250
	RETURN	Q	260
C		Q	270
	END	Q	280
	SUBROUTINE BLNCE (AIR,MFLO,CFR,SFLO,RMGFLO,CLH,CLO,CLH2O,MMMG,H2,H	Q	290
	12O,CO,CO2,O2,CH4,HMBE,OMBE)	R	10
	REAL MMMG,MFLO	R	20
C		R	30
C	ALL FLOW RATES ARE IN LB/HR. CALCULATE THE MOLAR FLOW RATES	R	40
C	OF HYDROGEN AND OXYGEN ATOMS INTO AND OUT OF THE REACTOR	R	50
C	IN LBMOLE/HR.	R	60
C		R	70
	HIN=MFLO*4.088/16.8+SFLO*2./18.+CFR*(CLH+CLH2O/9.)	R	80
	OIN=AIR*.42/28.84+SFLO/18.+CFR*(CLO+16.*CLH2O/18.)/16.	R	90
	HOUT=(RMGFLO/MMMG)*(2.*H2O+2.*H2+4.*CH4)	R	100
	OOUT=(RMGFLO/MMMG)*(H2O+2.*CO2+2.*O2+CO)	R	110
	HMBE=100.*(HIN-HOUT)/HIN	R	120
	OMBE=100.*(OIN-OOUT)/OIN	R	130
	RETURN	R	140
C		R	150
	END	R	160
		R	170

APPENDIX C. COAL ANALYSES

Proximate, ultimate and ash fusion analyses of the three coals burned in this investigation were performed by Commercial Testing and Engineering Company of Henderson, Kentucky. An ash fusion analysis was also performed on a sample composed of equal parts by weight of Rosebud and McKay subbituminous coals. The analyses are presented in Tables 17 through 20.

Table 17. Analyses of Rosebud Subbituminous Coal Used in Tests

(all values are percents on a weight basis except as noted)

PROXIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
% Moisture	13.99	XXXXX
% Ash	10.02	11.65
% Volatile	33.31	38.73
% Fixed Carbon	42.68	49.62
	<u>100.00</u>	<u>100.00</u>

ULTIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
Moisture	13.99	XXXXX
Carbon	58.54	68.06
Hydrogen	3.79	4.41
Nitrogen	0.82	0.95
Chlorine	0.01	0.01
Sulfur	0.93	1.08
Ash	10.02	11.65
Oxygen (diff)	11.90	13.84
	<u>100.00</u>	<u>100.00</u>

* FUSION TEMPERATURE OF ASH	<u>Reducing</u>	<u>Oxidizing</u>
Initial Deformation	2070 °F	2210 °F
Softening (H = W)	2100 °F	2240 °F
Softening (H = ½W)	2125 °F	2270 °F
Fluid	2180 °F	2360 °F

HIGHER HEATING VALUE (BTU/lb)	<u>As Received</u>	<u>Dry Basis</u>
	9900	11510

* H is cone height; W is cone width

Table 18. Analyses of McKay Subbituminous Coal Used in Tests
(all values are percents on a weight basis except as noted)

PROXIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
% Moisture	13.70	XXXXX
% Ash	11.24	13.02
% Volatile	31.31	36.28
% Fixed Carbon	43.75	50.70
	<u>100.00</u>	<u>100.00</u>

ULTIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
Moisture	13.70	XXXXX
Carbon	57.35	66.46
Hydrogen	3.63	4.21
Nitrogen	1.01	1.17
Chlorine	0.03	0.03
Sulfur	1.41	1.63
Ash	11.24	13.02
Oxygen (diff)	11.63	13.48
	<u>100.00</u>	<u>100.00</u>

FUSION TEMPERATURE OF ASH	<u>Reducing</u>	<u>Oxidizing</u>
Initial Deformation	2070 °F	2225 °F
Softening (H = W)	2100 °F	2260 °F
Softening (H = ½W)	2130 °F	2290 °F
Fluid	2185 °F	2360 °F

HIGHER HEATING VALUE (BTU/lb)	<u>As Received</u>	<u>Dry Basis</u>
	9759	11308

Table 19. Analyses of Indiana Bituminous Coal Used in Tests
(all values are percents on a weight basis except as noted)

PROXIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
% Moisture	15.33	XXXXX
% Ash	14.67	17.33
% Volatile	32.61	38.51
% Fixed Carbon	37.39	44.16
	<u>100.00</u>	<u>100.00</u>

ULTIMATE ANALYSIS	<u>As Received</u>	<u>Dry Basis</u>
Moisture	15.33	XXXXX
Carbon	55.54	65.60
Hydrogen	4.00	4.73
Nitrogen	1.07	1.26
Chlorine	0.02	0.02
Sulfur	2.88	3.40
Ash	14.67	17.33
Oxygen (diff)	6.49	7.66
	<u>100.00</u>	<u>100.00</u>

FUSION TEMPERATURE OF ASH	<u>Reducing</u>	<u>Oxidizing</u>
Initial Deformation	2070 °F	2180 °F
Softening (H = W)	2135 °F	2225 °F
Softening (H = ½W)	2185 °F	2310 °F
Fluid	2240 °F	2400 °F

HIGHER HEATING VALUE (BTU/lb)	<u>As Received</u>	<u>Dry Basis</u>
	10079	11904

Table 20. Ash Fusion Analysis of Rosebud-McKay Mixture

	FUSION TEMPERATURE OF ASH	
	<u>Reducing</u>	<u>Oxidizing</u>
Initial Deformation	2100 °F	2200 °F
Softening (H = W)	2130 °F	2230 °F
Softening (H = $\frac{1}{2}$ W)	2165 °F	2260 °F
Fluid	2200 °F	2300 °F

APPENDIX D. EXPERIMENTAL DATA

Experimental data from the coal combustion and gasification tests discussed in Chapter V are tabulated in this appendix. Table 21 includes the data from the extended coal combustion test and Table 22 lists the data from the fuel-rich gasification trials. A mixture of equal parts Rosebud and McKay subbituminous coals was used. The analyses of these coals are presented in Appendix C. The product gas analyses of Tables 21 and 22 were calculated via a dry basis analysis with water vapor found through an oxygen balance (see Appendix B).

Table 21. Extended Coal Combustion Test Data

Run No.	(A/F)/ (A/F) _S	Coal (lb/hr)	Primary Air Flow Temp. (lb/hr) (°C)	Secondary Air Flow Temp. (lb/hr) (°C)	Product Gas Flow Temp. (lb/hr) (°C)
30	1.20	19.8	21.4 50.	157. 185.	193. 1525.
31	1.22	19.8	21.3 54.	159. 174.	194. 1540.
32	1.21	19.8	21.3 56.	158. 171.	193. 1543.
33	1.40	19.8	20.7 51.	187. 167.	221. 1465.
34	1.45	19.8	20.7 56.	193. 161.	228. 1547.
35	1.28	19.8	20.8 56.	168. 161.	204. 1537.
38	1.14	13.2	23.1 26.	88.8 272.	122. 1373.
39	1.15	13.2	23.1 26.	90.6 269.	124. 1446.
40	1.44	10.2	22.9 26.	86.2 267.	117. 1330.
41	1.48	10.2	22.9 26.	88.8 265.	120. 1315.
42	1.45	15.0	22.7 26.	139. 265.	174. 1374.
43	1.45	15.0	22.6 27.	139. 263.	173. 1580.
44	1.26	15.2	22.8 27.	119. 291.	154. 1385.
45	1.27	15.2	22.9 27.	121. 291.	156. 1411.
46	1.23	10.0	23.4 28.	68.2 285.	100. 1418.
47	1.23	10.0	23.4 27.	68.3 292.	99.4 1435.
48	1.04	10.2	23.3 27.	55.6 234.	87.0 1504.
49	1.03	10.2	23.3 28.	54.6 225.	86.1 1510.
50	1.10	14.9	23.3 28.	98.3 196.	133. 1540.
51	1.10	14.9	23.3 26.	98.3 187.	133. 1567.
52	1.08	19.9	23.0 28.	137. 163.	176. 1580.
53	.990	20.1	22.9 27.	125. 193.	164. 1567.
54	1.48	10.0	23.3 27.	87.0 310.	118. 1340.
55	1.48	10.0	23.3 27.	87.0 311.	118. 1331.
56	1.28	10.0	23.4 27.	71.7 281.	103. 1329.
57	1.27	10.0	23.4 27.	71.4 259.	103. 1557.
58	1.07	10.0	23.4 26.	56.5 233.	87.6 1555.
59	1.06	10.0	23.4 26.	56.0 222.	87.6 1578.
60	1.46	15.0	23.2 26.	140. 196.	175. 1568.
61	1.49	15.0	23.2 26.	144. 173.	178. 1534.
62	1.24	15.0	23.2 26.	115. 163.	150. 1580.
63	1.23	15.0	23.2 24.	115. 160.	150. 1580.
64	1.07	15.0	23.1 24.	96.5 162.	131. 1553.
65	1.06	15.0	23.1 24.	95.2 164.	130. 1553.
66	1.07	19.9	22.9 24.	136. 162.	174. 1573.
67	1.08	19.9	23.0 23.	138. 156.	177. 1573.
68	1.23	19.9	22.9 24.	160. 145.	199. 1536.
69	1.23	19.9	23.0 23.	160. 140.	199. 1488.
70	1.42	19.9	22.8 23.	188. 174.	225. 1507.
71	1.44	19.9	22.8 23.	191. 192.	228. 1507.
72	.917	19.9	23.0 23.	113. 218.	151. 1554.
73	.901	19.9	23.2 23.	110. 231.	149. 1554.
74	.877	14.9	23.8 23.	74.1 244.	109. 1518.
75	.820	14.9	23.8 23.	67.5 243.	103. 1518.
76	.917	9.74	23.9 23.	42.6 217.	74.6 1518.
77	.909	9.74	23.8 23.	42.4 194.	74.1 1516.

Table 21. (continued)

Run No.	Product Gas Mole Fractions (%)					Hydr. Mass Balance Error (%)	Carbon Efficiency (%)	Heat Loss (%)
	H ₂ O	CO	N ₂	O ₂	CO ₂			
30	8.5	0.	73.7	4.4	13.5	-6.85	92.0	25.3
31	8.6	0.	73.7	4.5	13.3	-8.53	91.5	23.8
32	8.6	0.	73.6	4.5	13.3	-7.90	91.3	23.6
33	7.4	0.	74.3	7.3	11.0	-7.86	86.4	15.1
34	7.1	0.	74.5	7.0	11.4	-5.66	93.0	11.9
35	8.2	0.	73.9	4.9	13.0	-8.68	94.1	22.4
38	8.2	.6	73.4	4.4	13.3	2.34	90.1	32.1
39	7.3	1.2	73.6	4.2	13.7	11.5	97.9	28.9
40	6.4	0.	74.8	6.9	11.9	5.18	96.4	27.9
41	6.3	0.	74.8	6.9	11.9	3.91	98.5	29.2
42	9.2	0.	73.7	5.3	11.8	-38.9	97.0	35.8
43	8.3	0.	74.0	5.9	11.7	-24.6	95.7	19.0
44	6.9	.8	74.0	5.4	12.9	10.3	97.4	29.6
45	7.2	.7	74.0	5.3	12.9	4.95	97.5	29.3
46	7.1	.7	74.0	4.6	13.6	9.04	99.6	30.6
47	7.9	.4	73.7	4.6	13.3	-1.73	95.8	30.4
48	8.7	1.1	72.9	1.6	15.7	3.88	100.	34.6
49	8.8	1.3	72.8	1.5	15.6	3.66	100.	34.0
50	8.3	1.1	73.1	2.9	14.6	4.87	98.0	27.8
51	8.7	.8	73.1	2.8	14.6	-.58	96.2	27.1
52	8.0	1.2	73.2	2.5	15.1	10.1	100.	26.4
53	9.0	1.1	72.7	1.2	16.0	4.96	97.6	31.8
54	6.3	0.	74.8	7.3	11.6	4.50	95.9	26.8
55	6.8	0.	74.6	7.0	11.6	-4.27	95.9	29.3
56	7.8	.8	73.7	5.4	12.3	-4.11	94.3	32.2
57	7.6	.8	73.8	4.3	13.5	-.27	103.	24.7
58	8.4	1.1	73.1	3.2	14.2	5.59	93.7	25.2
59	8.5	1.4	72.9	1.4	15.8	4.10	105.	31.5
60	6.3	0.	74.8	6.1	12.8	6.07	104.	16.3
61	6.1	0.	74.9	8.2	10.8	7.04	89.5	5.3
62	7.4	.3	74.0	5.6	12.6	4.55	90.4	14.7
63	7.5	.7	73.8	4.6	13.4	3.71	98.4	19.5
64	9.9	.2	72.8	1.7	15.3	-11.9	94.9	32.5
65	10.3	.6	72.5	1.7	14.9	-15.7	94.2	32.1
66	8.7	.6	73.1	3.1	14.5	2.75	92.1	24.7
67	9.1	.7	73.0	1.5	15.8	-3.59	102.	32.4
68	8.2	.5	73.6	4.0	13.7	-5.51	99.5	25.3
69	7.9	.7	73.7	4.0	13.8	-1.24	101.	27.6
70	6.5	0.	74.7	7.2	11.6	4.45	92.1	13.1
71	6.3	0.	74.8	7.7	11.2	6.27	90.0	10.9
72	9.8	1.0	72.3	.9	16.0	4.75	90.4	31.8
73	9.9	2.0	71.8	.5	15.8	4.48	93.4	32.3
74	10.3	2.6	71.3	.3	15.5	2.44	93.3	33.3
75	10.1	4.7	70.5	.2	14.5	9.52	93.6	29.6
76	9.7	4.3	71.0	.3	14.7	3.53	103.	31.9
77	10.0	3.3	70.8	.2	15.1	-5.51	98.8	32.5

Table 22. Fuel-Rich Gasification Test Data

Run No.	(A/F)/ (A/F) _S	Coal (lb/hr)	Primary Air Flow Temp. (lb/hr) (°C)		Secondary Air Flow Temp. (lb/hr) (°C)		Product Gas Flow Temp. (lb/hr) (°C)	
96	1.27	10.2	22.5	10.	73.2	366.	104.	1421.
97	1.27	10.2	22.5	11.	73.4	378.	104.	1437.
98	1.28	10.2	22.8	11.	73.6	386.	104.	1466.
99	1.29	10.2	23.0	10.	73.8	391.	105.	1474.
100	1.30	10.2	23.1	10.	74.5	394.	106.	1475.
101	1.12	10.2	22.9	11.	61.3	389.	92.8	1545.
102	1.12	10.2	22.9	11.	61.1	385.	92.5	1541.
103	1.11	10.2	22.9	11.	60.9	382.	92.0	1554.
104*	1.11	10.2	22.9	11.	60.7	380.	91.8	1562.
105*	1.10	10.2	22.8	11.	59.7	378.	90.4	1560.
106*	.859	19.9	22.6	12.	105.	396.	141.	1584.
107	.860	19.9	22.2	10.	105.	399.	144.	1579.
108	.717	19.9	22.5	12.	83.7	390.	122.	1294.
109	.698	19.9	22.4	12.	80.9	384.	119.	1353.
110	.629	19.9	22.3	12.	70.8	378.	109.	1428.
111	.621	19.9	22.1	12.	69.8	376.	108.	1399.
112	.544	19.9	22.2	12.	58.2	371.	95.8	1329.
113	.544	19.9	22.4	12.	58.2	369.	96.1	1260.
114	.494	19.9	22.5	12.	50.6	301.	88.3	1237.
115	.501	19.9	22.6	12.	51.5	212.	88.8	1217.
116	.443	25.1	22.5	12.	60.0	235.	102.	1211.
117	.439	25.1	22.6	12.	59.3	280.	101.	1180.
118	.420	30.0	22.6	12.	70.8	328.	115.	1179.
119	.422	30.0	22.6	12.	71.3	348.	115.	1185.

*Not plotted due to excessive hydrogen mass balance errors

Table 22: (continued)

Run No.	Product Gas Mole Fraction (%)						Hydr. Mass Balance Error (%)	Carbon Efficiency (%)	Heat Loss (%)
	H ₂	H ₂ O	CO	N ₂	O ₂	CO ₂			
96	0.	9.4	0.	73.4	4.6	12.6	-24.8	91.3	34.5
97	0.	9.0	0.	73.6	4.5	12.9	-20.2	93.1	34.1
98	0.	8.6	0.	73.7	5.3	12.4	-14.1	89.7	28.7
99	0.	8.6	0.	73.7	4.9	12.8	-15.5	93.2	30.8
100	0	8.7	0.	73.7	5.1	12.5	-17.5	91.6	29.8
101	0.	7.0	2.5	73.1	3.7	13.6	17.9	103.	25.3
102	0.	9.5	1.5	72.6	2.4	14.1	-12.1	100.	33.3
103	0.	8.8	.7	73.1	2.9	14.5	-3.31	96.3	31.1
104*	0.	1.6	3.4	74.8	6.6	13.5	82.0	105.	9.4
105*	0.	3.1	2.2	74.7	6.6	13.4	65.4	95.4	11.2
106*	0.	2.1	3.2	74.2	7.3	13.2	81.3	79.7	6.4
107	.3	8.3	3.2	71.6	.2	16.4	20.6	98.3	32.1
108	1.7	7.8	7.4	68.7	.1	14.3	23.9	94.8	33.1
109	1.9	8.7	8.4	67.7	.1	13.2	15.9	93.0	29.7
110	3.1	8.5	11.3	65.5	.1	11.5	14.5	91.4	21.9
111	3.4	8.5	12.0	65.0	.1	11.0	12.5	91.9	21.9
112	4.9	8.6	14.3	62.6	.1	9.6	9.59	86.7	19.2
113	5.0	8.5	15.1	62.1	.1	9.1	8.46	88.6	20.4
114	6.3	8.2	16.8	60.4	0.	8.2	8.81	85.6	17.0
115	5.6	9.1	14.4	61.5	0.	9.3	7.86	80.6	19.1
116	8.1	7.4	17.5	58.7	0.	8.3	9.86	81.0	14.7
117	8.1	7.2	17.5	58.7	0.	8.4	12.1	81.0	15.6
118	9.0	7.4	16.6	58.2	0.	8.8	9.08	76.4	16.1
119	9.3	7.3	16.7	58.0	0.	8.7	7.22	77.2	15.9

*Not plotted due to excessive hydrogen mass balance errors

Table 22. (continued)

Run No.	Hot Gas Efficiency (%)	Cold Gas Efficiency (%)	Heating Value (BTU/scf)	Make Gas Yield (lb/lb coal)	Comb. Make Gas Yield (lb/lb coal)
96	----	----	----	---	----
97	----	----	----	---	----
98	----	----	----	---	----
99	----	----	----	---	----
100	----	----	----	---	----
101	----	----	----	---	----
102	----	----	----	---	----
103	----	----	----	---	----
104*	----	----	----	---	----
105*	----	----	----	---	----
106*	57.9	9.4	10.5	7.1	.212
107	62.4	10.4	11.1	7.2	.215
108	58.7	23.8	29.3	6.1	.444
109	63.3	26.6	33.2	6.0	.496
110	71.2	34.5	46.2	5.5	.624
111	72.4	36.8	49.6	5.4	.660
112	72.3	41.8	61.8	4.8	.718
113	72.9	44.3	65.1	4.8	.767
114	74.4	47.3	74.4	4.4	.797
115	68.4	40.8	64.5	4.5	.680
116	73.2	48.4	82.5	4.0	.768
117	71.5	48.1	82.8	4.0	.765
118	68.2	46.2	82.4	3.8	.701
119	69.6	47.5	84.0	3.9	.715

*Not plotted due to excessive hydrogen mass balance errors