MASTER

PULVERIZED FUEL COMBUSTION:
MODELING AND SCALEUP METHODOLOGIES

FIRST QUARTERLY REPORT
FOR THE PERIOD
19 SEPTEMBER 1980 - 31 DECEMBER 1980

PAUL F. LEWIS, THOMAS L. WOLF and ALAN GELB

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1. INTRODUCTION

This document is the first quarterly progress report on the effort for DOE to develop an understanding of the stability and carbon carryover characteristics of pulverized fuel combustors. This work is to be accomplished by improving and extending a model developed for entrained flow coal gasifier analysis by including a better description of the finite rate coal pyrolysis, pyrolysis product chemistry, char reactions, particle-particle interactions, radiative transport and recirculation/mixing.

The data to be analyzed with the model will include data from simple (cylindrical symmetry), geometry combustors with premixed and mixing reactants, swirl and recirculation. The analysis of these data with the model should lead to an understanding of the effects of fuel type, swirl, recirculation, O/F ratio and mixing rate on the location (stability) of the flame and the carbon carryover from the combustor.

The following sections describe the progress to date by task.

1.1 Data Collection and Screening

In this task PSI is collecting data from laboratory and small scale furnaces for comparison with the model. A large number of data reports have been identified¹⁻²¹ and various workers have been contacted in the search for additional information.

At the present time we have identified three sets of data for initial comparison of the model. The first is the cold flow data of Smoot and co-workers.^{19,20} This data comparison will allow major verification of the fluid mechanical aspects of the model without complication of chemical effects. The initial verification of the chemical model and radiative heat transfer model will be through comparison with the data of Cogoli et al.⁴ which was taken in a simple furnace on chars. Comparison with these data will allow partial verification of the model in simple flow without the complications of pyrolysis. The third set of data is that of Milne and Beachy.⁵ These data are for premixed coal air flames and will allow comparison of the model with coal combustion data taken in well defined laboratory tests without the effects of mixing.

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2. MODEL ELEMENT IMPROVEMENTS

The principal objective during this reporting period has been to outline and to begin to implement general features of the approach to combustor modeling so as to provide a framework for more detailed work to follow. Emphasis has been placed on upgrading the sophistication of our present model¹ in order to both include improved chemical models and take account of the effects of recirculation and swirl, while continuing to rely on the one-dimensional plug flow approach for reasons of simplicity and numerical tractability. The following subsections describe the progress by subtask.

2.1 Pyrolysis Model

The pyrolysis model is to be developed in such a way as to be consistent with the experimentally determined rates of pyrolysis and observed products as given by the work of at least Ubhayakar et al.,² Solomon et al.,³⁻⁷ and Suuberg.⁸⁻¹⁰ We have begun the process of developing the model by reviewing the recent literature starting with the review of Anthony and Howard¹¹ and including those works referenced above. Discussions with Drs. Suuberg and Solomon and Prof. Wendt at the University of Arizona were very helpful in defining the required level of model complexity. The approach is to make the model complete enough to give an adequate description of the evolution of the pyrolysis products yet simple enough to be computationally tractable.

The model of Suuberg for lignite pyrolysis fits this description reasonably well. A comparison of the models of Solomon and Suuberg indicates a great deal of mathematical similarity although the values of the constants are somewhat different. Solomon's correlation of products from various coals makes his model very attractive. It is clear that fluid mechanical processes and secondary reactions play a role under some conditions and, as Ubhayakar et al. suggest, cracking of larger volatiles to smaller molecules and soot is likely at high temperatures. This is consistent with the observation that tar yield changes with heating rate since cracking will be a function of residence time. For softening coals, fluid mechanical effects should affect

the pyrolysis rate and products. We have not yet included heating rate and softening effects in the model but have allowed for their future addition. Clearly, temperature is the dominant parameter in determining pyrolysis rate and product yield.

Two constraints that must be placed on any pyrolysis model are conservation of elemental mass and absence of dependence of the product distribution on a dry mineral matter free (DMMF) basis upon the mineral matter or moisture of the coal. Thus we base the model on the DMMF coal composition.

The pyrolysing structure is assumed to be describable by a set of measured constants which are the fraction of the DMMF coal which lead to various products with various rate constants. For example, there appear to be three processes which lead to CO_2 during pyrolysis. These three processes are represented by the amounts of CO_2 they can produce and the associated rate constants. Thus for one of these processes

$$\frac{dv_i(\text{CO}_2)}{dt} = (V_i^*(\text{CO}_2) - V_i(\text{CO}_2)) k_i(\text{CO}_2)$$

where $V_i^*(\text{CO}_2)$ is the mass fraction of the original DMMF coal which can produce CO_2 by this process, $k_i(\text{CO}_2)$ is the rate constant for the process and $V_i(\text{CO}_2)$ is the remaining portion of $V_i^*(\text{CO}_2)$. For a particle which started with mass M_o^k the rate of production of mass of CO_2 due to each of these processes is

$$\frac{d\text{CO}_2}{dt} = (V_i^*(\text{CO}_2) - V_i^k(\text{CO}_2)) M_o^k$$

$$(1 - f_{\text{ash}} - f_{\text{wet}}) k_i(\text{CO}_2)$$

where f_{ash} and f_{wet} are the as received mass fractions of ash and moisture in the coal. It is therefore convenient to define

$$W_i^k(\text{CO}_2) = V_i^*(\text{CO}_2) M_o^k (1 - f_{\text{ash}} - f_{\text{wet}})$$

This allows us to write

$$\frac{dw_i^k(\text{CO}_2)}{dt} = (w_i^{*k}(\text{CO}_2) - w_i^k(\text{CO}_2)) k_i^k(\text{CO}_2)$$

and the molar production rate of CO_2 due to the three processes from a particle of size class k is then

$$\frac{d\text{CO}_2}{dt} = \frac{1}{44} \sum_{i=1}^3 \frac{dw_i^k(\text{CO}_2)}{dt}$$

Similar equations apply to other pyrolysis products.

The above description applies to parallel (non-competitive) reactions. The extent to which competitive reactions occur is not clear but it appears that the major effect of competitive reactions, including heating rate, is in modification of the hydrocarbon fraction of pyrolysis products. Thus a model for cracking of pyrolysis products before they escape from the particle could alter W^* for the appropriate products or change the product without changing the W^* . For example, cracking of butane to acetylene on a particle surface,

would lead to additional H_2 production whereas cracking of acetylene to methane with hydrogen abstraction

would deplete the hydrogen in the coal and change $W^*(\text{H}_2)$. Although we have not yet included these processes in the computer model, we describe them to show that they are easily added to the proposed mathematical model of pyrolysis.

The V_i^* and k_i for most of the pyrolysis products are obtained from experimental data such as those of Suuberg for CO_2 , CO , CH_4 , C_2H_4 , and H_2 . However, several of the V_i^* and k_i are obtained by different means as described below. There appear to be two components which produce H_2O moisture and hydroxyl. The moisture portion is

$$V_1^*(\text{H}_2\text{O}) = f_{\text{wet}} / (1 - f_{\text{wet}} - f_{\text{ash}})$$

The other fraction is determined by oxygen balance from

$$V_2^*(\text{H}_2\text{O}) = \frac{18}{16} \left\{ \text{DMMF}(\text{O}) - \frac{32}{44} \sum_i V_i^*(\text{CO}_2) - \frac{16}{28} \sum_i V_i^*(\text{CO}) \right\}$$

The rate constant $k_2(\text{H}_2\text{O})$ is taken from Suuberg whereas $k_1(\text{H}_2\text{O})$ is large but as yet undetermined.

The current thinking is that nitrogen is released in two stages, primarily as HCN . Although much research is continuing in the pyrolysis of fuel nitrogen, a definitive model is not yet available. We have for the present split the fuel nitrogen equally between the two components and taken the relative rates of the two processes as determined by Solomon but scaled to Suuberg's rate for the hydroxyl H_2O component. Thus

$$V_1^*(\text{HCN}) = V_2^*(\text{HCN}) = \frac{1}{2} \frac{27}{14} \text{DMMF}(\text{N})$$

The sulfur component appears to pyrolyze primarily as CS_2 . For this process we have taken the rate for the second stage CO_2 process from Suuberg with

$$V_1^*(\text{CS}_2) = \frac{76}{64} \text{DMMF}(\text{S})$$

We determine the final hydrocarbon component from hydrogen balance

$$\begin{aligned} H_{\text{excess}} = & \text{DMMF}(\text{H}) - \frac{4}{16} \sum_i V_i^*(\text{CH}_4) - \frac{4}{28} \sum_i V_i^*(\text{C}_2\text{H}_4) \\ & - V_1^*(\text{H}_2) - \frac{1}{27} \sum_i V_i^*(\text{HCN}) \end{aligned}$$

The composition of this product is not well determined, is generally described as tar and has an atomic C/H ratio of about unity. For simplicity and initial implementation we have assumed that this hydrogen produces C_2H_2 in three steps with 20% in the first step and 40% in each of the next two steps with the rates as determined by Snuberg for "other HC" and the two tar components respectively. Thus

$$\sum_{i=1}^3 V_i^* (C_2H_2) = 13 H_{\text{excess}}$$

A summary of this first pass pyrolysis model for Montana lignite is given in Table 2.1. The coal composition is given in Table 2.2. All of the information in the tables is input to the computer code. In this model, we have taken the pyrolysis process to change the particle size in a constant manner, that is

$$\frac{d\phi^k}{dt} = \alpha \frac{(1 - \phi^k)}{M^k} \left. \frac{dM^k}{dt} \right|_p$$

where ϕ is the porosity of the particle and $\left. \frac{dM^k}{dt} \right|_p$ is the rate of particle mass loss due to pyrolysis. If α is greater than unity the particle increases in diameter during pyrolysis and if α is less than unity, the particle shrinks. Lacking definitive information we will initially take an α of unity.

2.2 Reactions of Pyrolysis Products

In this subtask we are developing a model for the chemical reactions of volatile products. Indications are that the products are all released from the particles as gases, although, because of the nature of experiments, this is difficult to observe. The approach we have taken is to use a modified quasi-global mechanism which uses global rates for the reactions of C_3 and higher hydrocarbons to form smaller molecules and to use detailed kinetics for the C_2 and smaller molecules. A similar approach has been taken by several workers. However, they have taken global rates for the reaction of hydrocarbons to form primarily CO and H_2 . This approach has

TABLE 2.1

SUMMARY OF PYROLYSIS MODEL FOR MONTANA LIGNITE

Molecule	V*	Rate ^a	
		log A	E
CO ₂	0.0684	11.33	36.2
	0.0324	13.71	64.3
	0.0131	6.74	42.
CO	0.0212	12.26	44.
	0.642	12.42	59.5
	0.0271	9.77	58.4
CH ₄	0.0041	14.21	51.6
	0.0110	14.67	69.4
C ₂ H ₄	0.0018	20.25	74.8
	0.0049	12.85	60.4
H ₂	0.0060	18.20	88.8
H ₂ O	b	c	c
	d	13.9	51.4
HCN	e	13.9	51.4
	e	14.2	61.4
CS ₂	f	13.71	64.3
C ₂ H ₂	g	16.23	70.1
	h	11.88	37.4
	h	17.3	75.3

a $k = A e^{-E/RT}$
 $R = 1.987 \times 10^{-3}$ kcal/mol-K

b moisture

c rate large but as yet undetermined

d determined from oxygen balance

e 1/2 of the fuel nitrogen forms each component

f determined from non-mineral sulfur

g determined from 20% of excess hydrogen

h determined from 40% of excess hydrogen

TABLE 2.2

COMPOSITION OF MONTANA LIGNITE

Dry mineral matter free elemental analysis, DMMF

Element	Mass Fraction
C	0.7119
H	0.0456
N	0.0108
S	0.0132
O	0.2185

As received analysis

Moisture	6.8%
Ash (mineral matter)	9.9%

been reviewed recently by Dryer and Glassman.¹² The chemistry of species up to C₂ hydrocarbons is reasonably well verified for combustion conditions. The latest available rate information is part of the PSI computer code.¹ In future work we will be developing global rates for the breakup of the larger hydrocarbons.

2.3 Heterogeneous Chemistry

In this subtask the hope is to develop a self-consistent description of the reactions of coal char with O₂, CO₂, H₂O, O and OH. Several studies have shown substantial similarities between the rates of reaction of these species. We hope to exploit these similarities to develop a combined mechanism which will properly describe the reaction in the presence of mixtures of the reactant gases.

The previous model¹ for the heterogeneous reactions was

where C_f is a vacant active site, C is any carbon and C(X) is an X molecule adsorbed on an active site. By modifying the oxygen adsorption step to

the same form for the oxygen reaction rate is found but the interpretation becomes altered. The surface reaction rate, k_6 , could be very fast and could account for the observation that oxidation is about five orders of magnitude faster than gasification and becomes so by causing a much higher surface coverage, $C(O)$. The rate of the common desorption step would be increased by this higher coverage. The oxygen atom reaction could be

and is very fast. Thus we hope to find a surface species common to the above reactions. In addition, the observation that CO_2 may be a major product of oxidation could be explained by there being a commonality to the processes by

Because large concentrations of hydroxyl radical are often present in combustors, well above equilibrium levels, we are also planning to include the hydroxyl reaction with the surface. It is possible that there is some common step between the hydroxyl and steam reaction and this aspect will be exploited. Meanwhile the existing reaction mechanism¹ will be used.

2.4 Particle-Particle Interactions

To a first approximation particulates move at a uniform velocity u_p , which is not necessarily equal to the gas velocity u . In previous work drag and inertial forces were equated for each particle size classification, yielding a range of particle velocities u_p^K . However, it is more correct to assume that there are sufficient particle-particle collisions to enforce a uniform velocity for all particles, and to evaluate this velocity by balancing drag and inertial forces for the entire particulate cloud. This conclusion is indicated by an estimation of the particle-particle collision rate, based on simple kinetic theory, in which the magnitude of turbulent fluctuations of particle and gas velocities are assumed equal. For typical gasifier operating conditions, this calculation establishes that each particle will experience several collisions during its residence time in the combustion chamber. This conclusion then leads to a particle momentum equation

$$u_p \frac{du_p}{dx} = \sum n^K D^K / \sum n^K m_p^K$$

where

$$D^K = (u - u_p) \left\{ 3\pi\mu d^K + \frac{\pi}{20} \rho d^{K^2} |u - u_p| \right\}$$

Symbols are defined in Sec. 2.6.

Deviations from this mean particle velocity resulting from the fact that the drag on various particle sizes differs can then be treated as a perturbation. This effect will be addressed in future work.

2.5 Radiative Transport

No work has been performed on this subtask during the reporting period.

2.6 Recirculation Mixing

For geometries relevant to the present program, simplification of the flow equations is afforded because complex multidimensional fluid mechanics,

which impact the formation of radial temperature gradients, do not appear to be strongly coupled with complex chemistry. In the inlet vicinity where swirl and recirculation are of primary importance, temperatures are sufficiently low that reaction rates are not highly dependent on the details of the temperature profile. Also, the essential features of the flow geometry are not expected to be strong functions of chemistry, but more directly influenced by such parameters as gasifier inlet geometry, gas flow rate, and particulate loading. Farther downstream where gas temperatures are higher and reaction rates are more sensitive to temperature, the 1D plug flow approximation is more appropriate.

These considerations have suggested a decoupled calculation in which the details of the velocity field are computed independently of detailed chemistry, although perhaps subject to some approximate prescription of source terms for mass and energy. On the basis of this 2D calculation boundaries for recirculation regions can be roughly defined, and mass transfer rates across these boundaries can be estimated. We will make the usual approximation that recirculation zones are fully mixed, and that the non-recirculating regions can be treated using the 1D plug flow approach, now with a prescribed rate of mass transfer and variable flow area.

At present the revised 1D conservation equations have been incorporated into the computer code, and 2D flow modeling is scheduled to receive immediate attention during the next quarter.

Conservation equations for 1D gas-particle flow were developed in detail in ref. 1, and in the present study extensive use will be made of this work. However, important simplifications have been indicated by recent work, and recirculation and swirl introduce some additional terms. Also, numerous notational changes have been introduced in order to cast the equations in a more convenient and computationally tractable form. For these reasons, a revised system of 1D conservation equations is presented in this section.

A simplifying approximation has been introduced in connection with the present work. Gas pressure has been assumed constant, eliminating the need to integrate a gas phase momentum equation. This approximation is well supported for one-dimensional treatment of low Mach number flows, although it

will not be invoked in the two-dimensional fluid dynamic model to be developed later in this program.

With these simplifications, the steady 1D conservation equations in the plug flow region are written as follows:

- Gas Phase Equations:

$$\text{Continuity: } \frac{d}{dx} (\rho u A) = \dot{M}_R + A \sum_K \dot{m}_n^K$$

$$\text{Conservation of Species } j: \frac{d}{dx} (\rho u Y_j A) = \dot{M}_{jR} + A \sum_K \dot{m}_j^K + A W_j \dot{\chi}_j$$

$$\begin{aligned} \text{Conservation of Energy: } \rho u c_p \frac{dT}{dx} = & \sum_K \sum_j n_j^K c_{p_j} (T^K - T) \\ & + \frac{1}{A} \sum_j \dot{m}_{jR} c_{p_j} (T^K - T) \\ & + \sum_K n_j^K \dot{q}_c^K + \dot{q}_{gc} \end{aligned}$$

$$\text{Equation of State: } \rho = \frac{p \bar{W}}{RT}, \text{ where } \bar{W} = \left(\sum_j \frac{Y_j}{W_j} \right)^{-1}$$

- Particle Phase Equations: (K=0, 1, 2 ... N)

$$\text{Continuity of Particle Flux: } \frac{d}{dx} (n^K u_p A) = 0$$

$$\text{Conservation of Mass: } u_p \frac{dm_p^K}{dx} = \dot{m}^K$$

Conservation of Momentum: $\sum n^K D^K = u_p \frac{du_p}{dx} \sum_K n^K m_p^K$

where $D^K = (u - u_p) \left\{ 3\pi \mu d^K + \frac{\pi}{20} \rho d^{K^2} |u - u_p| \right\}$

Conservation of Energy: $u_p m_p^K c_p^K \frac{dT^K}{dx} = - \sum_j \dot{m}_j^K c_{p_j} (T^K - T)$

$$- \dot{q}_c^K + \dot{q}_{ch}^K$$

$$+ \dot{q}_{rf}^K + \dot{q}_{rw}^K + \dot{q}_{rp}^K$$

Variable definitions are as follows:

A	= plug flow area (cm^2)
c_{p_j}	= heat capacity of species j (erg/g K)
c_p	= bulk heat capacity of gas mixture (erg/g K)
c_p^K	= effective heat capacity of particle (erg/g K)
d^K	= particle diameter (cm)
D^K	= fluid dynamic drag acting on particle (dynes)
K	= superscript denoting particle size classification
$\dot{m}^K$	= mass transfer rate from particle to gas (g/s-part)
$\dot{m}_j^K$	= mass transfer rate from particle to gas of species j (g/s-part)
$\dot{M}_R$	= local mass transfer rate from recirculation region to plug flow (g/s-cm)
$\dot{M}_{jR}$	= local mass transfer rate from recirculation region to plug flow of species j (g/s-cm)
m_p^K	= particle mass (g)
n^K	= particle number density (part/cm ³)
p	= pressure (atm)
$\dot{q}_{cg}$	= volumetric energy release from gas phase chemistry (erg/sec-cm ³)
$\dot{q}_c^K$	= heat conduction rate from particle to surrounding gas (erg/s-part)
$\dot{q}_{rf}^K$	= radiative energy transfer rate from flame to particle (erg/s-part)
$\dot{q}_{rp}^K$	= radiative energy transfer rate from other particles to particle (erg/s-part)
$\dot{q}_{rw}^K$	= radiative energy transfer rate from walls to particle (erg/s-part)
$\dot{q}_{rR}^K$	= radiative energy transfer rate from recirculation zones to particle (erg/s-part)
$\dot{q}_{ch}^K$	= heat release rate per particle from heterogeneous chemistry (erg/s-part)

R = universal gas constant ($\text{cm}^3\text{-atm/mole-K}$)
 u = gas velocity (cm/s)
 u_p = particle velocity (cm/s)
 $\bar{W}$ = avg. molecular weight of gas mixture (g/mole)
 W_j = molecular weight of species j (g/mole)
 Y_j = mass fraction of species j in gas phase
 μ = gas mixture viscosity (poise)
 ρ = gas mixture density (g/cm^3)
 $\dot{X}_j$ = volumetric molar production rate of species j from gas phase chemistry (moles/cm^3)

All of the terms appearing in the 1D conservation equations can be calculated using the present model, except those identified with mass and energy transfer from the recirculation zone. These additional quantities will be computed through application of the 2D fluid mechanics model. Also, estimation of some quantities will be refined in connection with the present program, e.g. pyrolytic mass transfer from particulates and radiative energy transfer terms.

2.7 References

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3. DATA ANALYSIS

No work has been performed on this task during the reporting period.

4. SCALING LAWS

No work has been performed on this task during the reporting period.