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1991

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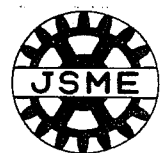
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YASUO KUROSAKI — JSME

RENO, NEVADA
MARCH 17-22, 1991

THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
UNITED ENGINEERING CENTER
345 EAST 47TH STREET
NEW YORK, N.Y. 10017



THE JAPAN SOCIETY OF MECHANICAL ENGINEERS
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THREE-DIMENSIONAL SIMULATION OF COAL BURN-OFF UNDER AIR-STAGED CONDITIONS

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ABSTRACT

Three-dimensional computer simulation of coal particle combustion have been carried out using new combustion models incorporated with FLUENT, a commercially available simulation code.

The results of carbon burn-out from simulation indicate good agreement with experimental results in a laboratory scale coal combustor even at the final stage of combustion, in which unburned carbon ratio is as low as a few percents.

Effects of staging-air velocity on carbon burnout is then studied by using developed simulation code. Simulation reveals that the velocity, as well as the amount and the injecting point of staging-air, is an important factor in carbon burnout. The validity of the simulation is confirmed with experimental data.

NOMENCLATURE

Symbols	Units	
a	m ² /kg	Specific surface area
A	s ⁻¹ or kg/m ² s(atm) ⁿ	Frequency factor
E	kJ/mol	Activation energy
k	s ⁻¹ or kg/m ² s(atm) ⁿ	Reaction rate coeff.
L	m	Length of the combustor
m	kg	Component mass
n	-	Order of reaction
PO ₂	atm	Partial pressure of O ₂
r	kg/m ² s	Rate of reaction
R	J/mol K	Gas constant
T	K	Temperature
t	s	Time
v	-	Yield volatile
v*	-	Volatile yield ultimately
x	m	Axial distance

Subscripts

c	Char
p	Particle
v	Volatiles

INTRODUCTION

Pulverized coal is widely used for coal fired boilers which generate steam for utilities and industries. Since little domestic resource forces Japan to import coal from the coal producing countries all over the world. Coal quality differs substantially from mine to mine and coal to coal, even seam to seam. It is difficult to burn efficiently coal of wide variety, in one boiler meeting stringent environmental regulations. Therefore, technologies to find out the best suited operating condition of a boiler for each coal are desirable.

Computer simulation can be one of the possibilities to develop these technologies. Computer simulation, which is able to predict carbon burnout and NOx emission, would show the best suited operating conditions to a coal without taking the risk to actually burn the coal in the boiler only finding it produces too much unburned carbon and/or NOx under some conditions.

Now there are some general-purpose simulation codes available, which can simulate heat and fluid dynamics during coal combustion. As for pulverized coal combustion, some applications can be found in the literature (1,2). Truelove predicted gas velocity profiles, gas temperature profiles and O₂ concentration distributions in near burner region in a cylindrical laboratory scale combustor assuming axisymmetry. He provided experimental data to be compared with the prediction. Visser and Weber modified Truelove's model and simulated gas temperature profiles and concentration distributions of O₂, CO and CO₂ in also near burner region in a

cylindrical laboratory scale combustor assuming axisymmetry. They also provided experimental data.

While gas phase properties have been extensively studied and successfully predicted, no reports dealing with solid phase properties, notably carbon burnout, are available in the literature. In addition, axisymmetry has been assumed in those studies, making the flowfield relatively simple pseudo two-dimensional, despite simulation of commercial boilers is more complicated and required to be three-dimensional.

In previous works (3-5), there are some reports dealing with simulation of commercial boilers. Abbas and Lockwood, and Fivelland and Wessel too, applied their simulation code to a commercial boiler; however, verifying data are unavailable. Boyd and Kent actually measured gas temperature profiles in a commercial boiler with a suction pyrometer to be compared with their prediction. However, the model seemed to fail to predict the profiles precisely.

In this study, the objective is to develop a computer code able to predict particle phase properties, carbon burnout profiles to be precisely, in a three-dimensional flowfield, namely, a flowfield of air-staged combustion in a laboratory scale combustor.

MATHEMATICAL MODELS

Heat and Fluid Flow Models

Two-phase turbulent swirling flow-fields in a laboratory scale combustor is calculated by the FLUENT (6) code.

In FLUENT, basic equations for the continuous gas phase are time-mean equations of conservation of mass, momentum, energy, and chemical species and expressed in the form of the Eulerian formulae. On the other hand, the momentum equation of particles is solved in the Lagrangian frame of reference. Two phases are coupled through source terms in the Eulerian equations.

Turbulence is calculated with the two-equation $k-\epsilon$ model. The eddy-dissipation combustion model is used for gas-phase reaction, assuming gas mixing rate control the reaction. A flux method is applied to radiative heat transfer in the flame.

The interactions between continuous gas phase and discrete particle phase are computed by a particle source in a cell method.

Coal Combustion Models

The coal combustion process can be divided into two parts: devolatilization of coal particles and following heterogeneous char combustion.

Widely used coal combustion models are Ubhayakar et al.'s devolatilization model (7) and Field et al.'s char combustion model (8), which takes into account diffusion of O_2 to the surface of char particles and chemical reactions on the surface. While the models successfully predicts carbon burnout at the late stage of combustion, as well as gas phase properties, in relatively simple flowfields, they cannot predict carbon burnout accurately in complex flowfields such as that of air-staged combustion.

Models selected for this study are simple phenomenological models describing the behavior of coal particles: rapid weight loss through

devolatilization, followed by slow weight loss through char combustion.

Devolatilization model. Krevelen et al.'s model (9), which is a simple, single-step first order reaction model, is selected for devolatilization of coal particles. Since devolatilization time is very short compared to particle residence time in furnaces, development of more sophisticated devolatilization model is unlikely to improve overall performance significantly.

The rate of devolatilization is described by

$$\frac{dV}{dt} = k_v (V^* - V) \quad (1)$$

where k_v is the rate constant expressed in the Arrhenius form, and V^* is the amount of ultimate volatile yielded from a coal particle. Both values are experimentally decided by using an electrically heated drop tube furnace.

k_v is assumed to be constant over different coals, because difference in k_v among coals is found to be small and therefore has insignificant effects on carbon burnout at the char combustion stage. Kinetic parameters for k_v used in this study are: frequency factor $A_v = 2.0 \times 10^3 [s^{-1}]$ and Activation energy $E_v = 73.6 [kJ/mol]$.

On the other hand, V^* varies substantially from coal to coal, having significant effects on carbon burnout of each coal. Note that V^* is the amount of volatile yielded under combustion conditions and therefore would be larger than proximate volatile matter. V^* in this study is measured weight loss of coal during devolatilization in the drop tube furnace at 1773 K.

Char combustion model. A theoretical model based on diffusion of O_2 to the surface of particles and chemical reactions on the surface has been widely used to simulate coal combustion. While the model works well to predict gas phase properties such as gas velocities, gas temperatures and major chemical species in gas phase, it fails, for example, to predict solid phase properties, carbon burn-out for one, especially at the late stage of combustion.

The model chosen over a number of models to predict carbon burn-out is that of Sadakata et al (10). In the model, the rate of char combustion is described as:

$$\frac{dm_c}{dt} = -r_c a m_c \quad (2)$$

$$r_c = k_c P_{O_2}^n, n = 0.5 \quad (3)$$

The rate constant is expressed in the Arrhenius form:

$$k_c = A_c \exp(-E_c / RT_p) \quad (4)$$

Char combustion is carried out in the drop tube furnace to experimentally determine the parameters. The apparent reaction order of O_2 is found to be 0.5 over char combustion with O_2 concentrations ranging from 3 to 21 vol%. The kinetic parameters for the

char reaction rate coefficient, A_c and E_c , are determined through experiments at temperatures ranging from 1273 to 1673 K.

NUMERICAL SOLUTION

Coal combustion sub-programs are developed based on selected models and incorporated into FLUENT.

In order to analyze a cylindrical laboratory scale combustor, the governing equations are expressed in cylindrical coordinates. The computational domain of the combustor is divided into 33, 17, and 17 elements in x , r , and θ directions respectively.

Particle size distributions are approximated by histograms of five representing diameters. A set of Lagrangian particle trajectory equations for a particle of each representing diameter is solved every ten iterations of gas phase computation. Dividing the burner of the combustor into eight parts, coupled with five representing particle diameters, requires computation of 40 different cases for particle phase.

It typically requires 1500 iterations to obtain a converged solution.

EXPERIMENTAL

In order to evaluate the performance of the simulation code, experiments are carried out in a laboratory scale coal combustion furnace.

Experimental facility

Schematic diagram of the laboratory scale coal combustor used in this study is shown in Fig.1. The combustor is 0.3m in diameter and has an effective length of 2.5m. The furnace has a burner at the top and 17 air-injection ports for air-staged combustion and 17 sampling ports along itself.

Figure 2 shows the burner section of the furnace. It is a single burner system which provides swirling secondary air as well as pulverized coal entrained by primary air. It produces a stable diffusion flame downward.

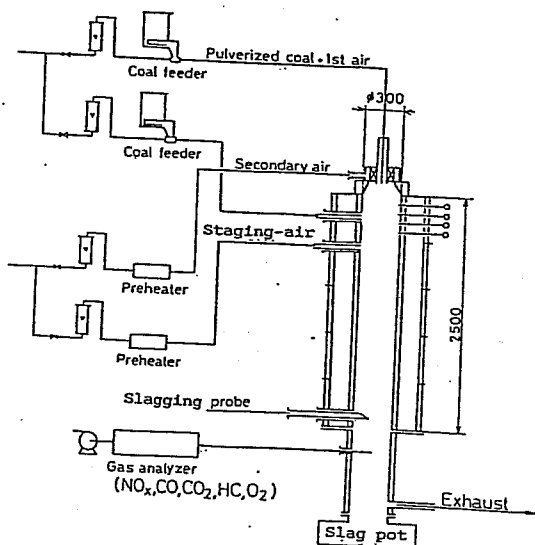


Figure 1. Schematic diagram of the laboratory scale coal combustor.

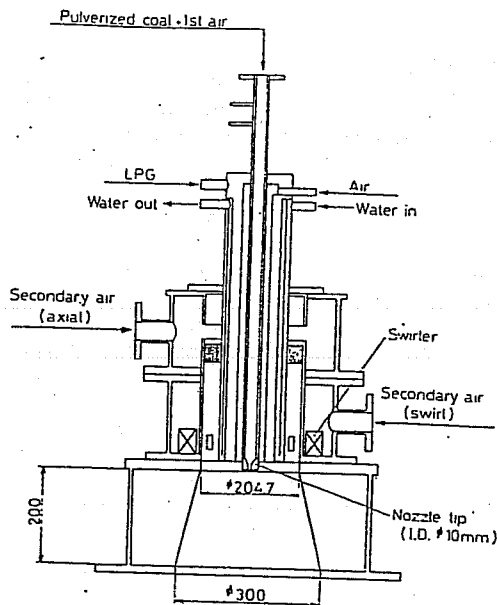


Figure 2. Detail of the swirl-type burner

All operating conditions are the same through out the experiments except the position, the rate and the velocity of the staging air. Coal is pulverized until all coal particles are smaller than $150 \mu\text{m}$ and 80% of them are smaller than $74 \mu\text{m}$. Coal feed rate is about 6kg/hr, which will yield O_2 concentration of 4% at the end of the combustor with total air flow of $52\text{Nm}^3/\text{hr}$. The secondary air and the staging air flows are preheated to 623K while the primary air of room temperature enters the combustor.

Char particles are sampled to measure carbon burn-out at various stages of combustion. A water cooled sampling probe is used. Sampling ports are located every 0.15m along the combustor.

Coal Properties

Proximate and Ultimate analyses of two bituminous coals used in this experiment, high volatile coal, AC, and medium volatile coal, AD, are listed in TABLE 1.

TABLE 1 Coal properties

Property	Coal	
	AC	AD
Proximate analysis		
Moisture, %	4.9	2.4
Ash, %	15.9	14.1
Volatile matters, %	35.9	26.4
Fixed carbon, %	45.3	57.1
Ultimate analysis		
C, %	81.9	85.6
H, %	6.3	5.4
O, %	9.7	7.0
N, %	1.6	1.9
S, %	0.51	0.44
Calorific value, MJ/Kg	26.9	28.4

RESULTS AND DISCUSSION

Coal Burn-out Profiles

Figures 3 and 4 show comparison between calculated and measured carbon burn-out profiles along the combustor. The calculated carbon burn-out shown is cross sectional average of unburned carbon over a number of particles.

Calculated carbon burn-out profiles agree reasonably well with measured ones under air-staged conditions. Unburned carbon decreases gradually till staging-air is introduced, representing slow combustion in fuel rich zone. Then it decreases rapidly after the staging-air port, because staging-air provides fresh oxygen and thus promotes combustion.

Developed computer code gives reasonably accurate predictions of carbon burn-out profiles even at the late stage of combustion under staging-air, which makes flowfields three-dimensionally complicated.

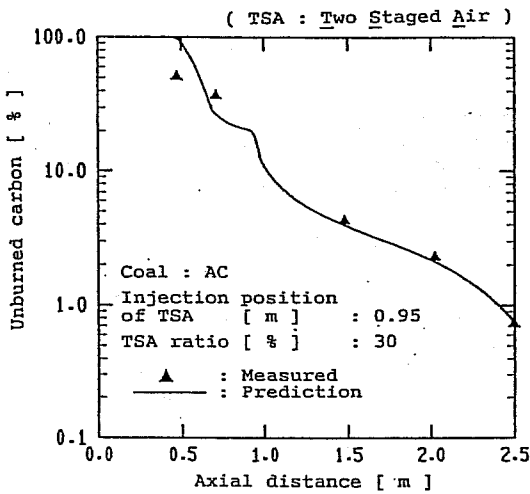


Figure 3. Comparison of coal burnout profiles measured and predicted for AC coal.

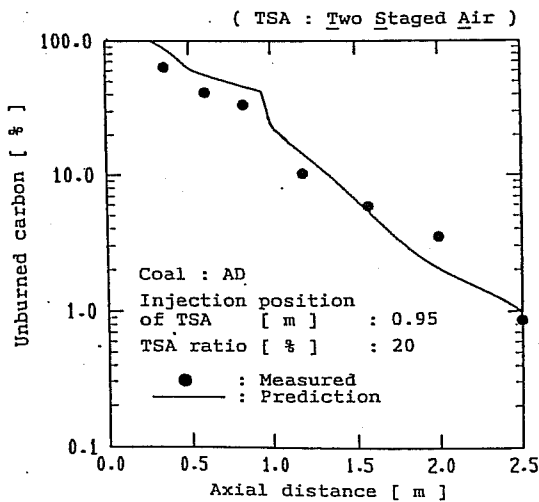


Figure 4. Comparison of coal burnout profiles measured and predicted for AD coal.

Effects of Staging-Air Velocity

Effects of the inlet velocity of staging air is then studied with the computer code and the laboratory scale combustor.

Air-staged combustion is widely used to reduce NOx emission. Effects of the amount and the injecting point of staging-air on combustion have been well studied. It is generally said that injecting more staging-air later yields less NOx but, at the same time, more unburned carbon.

However, an interesting phenomenon was found in a commercial boiler: increasing staging-air lowered not only NOx emission but also unburned carbon. Increased inlet velocities of staging-air are possibly responsible for the simultaneous decrease in NOx emission and unburned carbon.

Comparison of prediction and measurement. The cases studied in this study are:

Case 1 : staging-air is injected from one side at high velocity (14m/s)

Case 2 : staging-air is injected from opposing two sides at low velocity (1.8m/s)

The inlet velocity is varied by changing the injection port in diameter to keep the amount of staging air constant.

Predicted and measured unburned carbons are compared at the end of the combustor in Fig.5. The computer code predicts reasonably well the phenomenon that, regardless of the injection points, the higher inlet velocity yields lower unburned carbon at the end of the combustor.

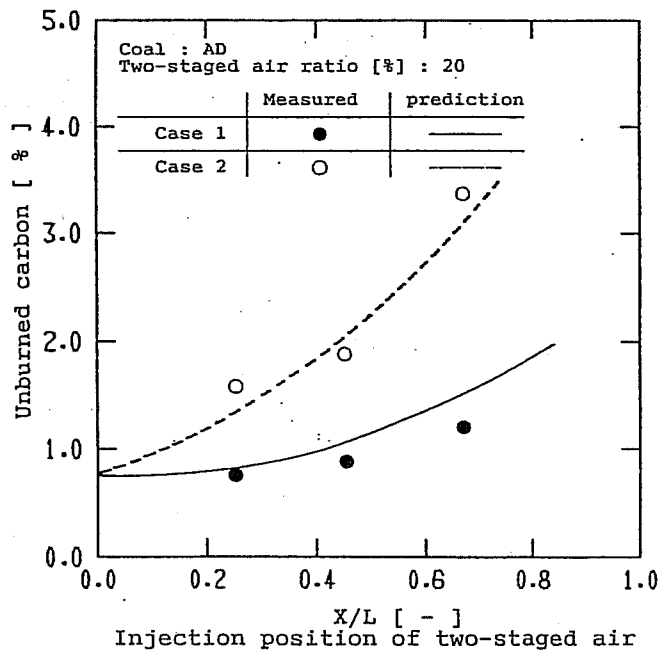
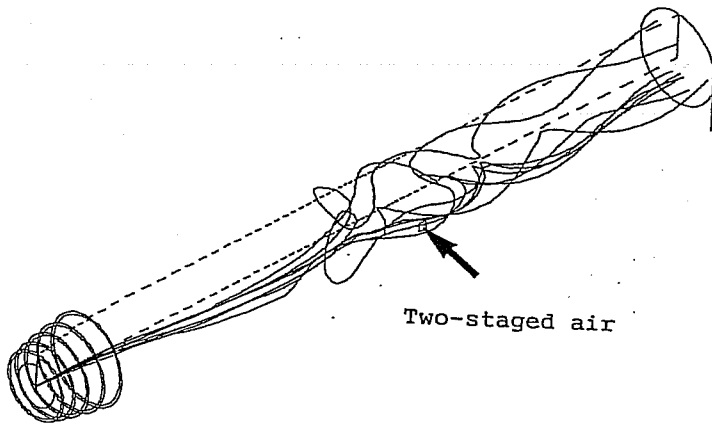


Figure 5. Effect of inlet velocity on unburned carbon.

Analysis. The phenomenon is then analyzed with the simulation code.

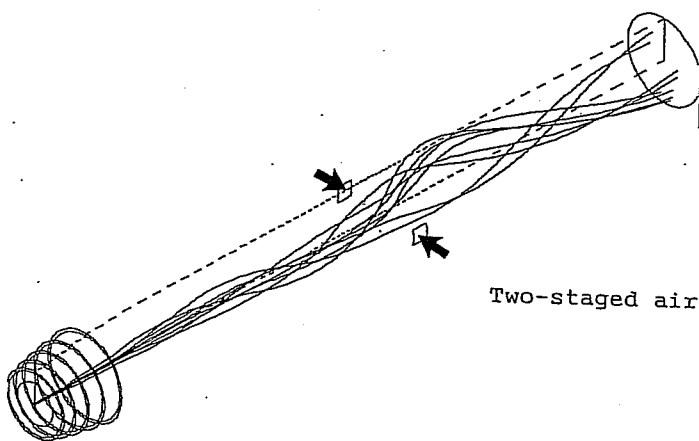
Figures 6 and 7 show particle trajectories in cases 1 and 2 respectively. Particle trajectories around the staging-air injection port in case 1, i.e. higher inlet velocity, are more disturbed than those in case 2, i.e. lower inlet velocity.

Particle residence time distributions in case 1 and 2 are shown in Figs.8 and 9. The shift in the distribution indicates that residence time in case 1 is longer than that in case 2. Difference in mean residence times in cases 1 and 2 is 0.2 seconds large enough to have noticeable effects on unburned carbon.



Case 1 : Two-staged air injected from one side at high velocity (14m/s)

Figure 6. Particle trajectories
(Representative diameter : $60\mu\text{m}$)



Case 2 : Two-staged air injected from both sides at low velocity (1.8m/s)

Figure 7. Particle trajectories
(Representative diameter : $60\mu\text{m}$)

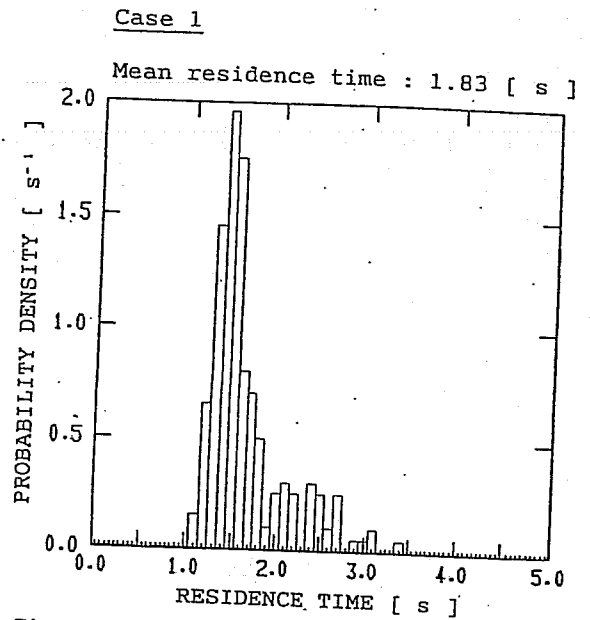


Figure 8. Particle residence time distribution in Case 1.

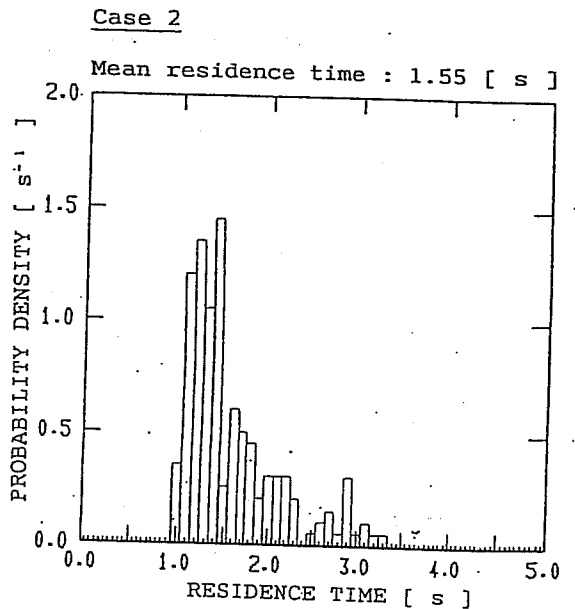


Figure 9. Particle residence time distribution in Case 2.

Computer simulation reveals that the higher inlet velocity gives better mixing around the staging-air injection port, resulting in longer particle residence time, thus lower unburned carbon.

CONCLUSION

Coal combustion sub-programs are developed based on selected devolatilization and char combustion models. The programs, coupled with FLUENT, successfully predict unburned carbon profiles through three-dimensionally complex flowfields under air-staged conditions in a laboratory scale coal combustor.

Effects of the inlet velocity of staging-air on unburned carbon at the end of the combustor is then studied with the computer code. The inlet velocity has noticeable effects on unburned carbon: The higher an inlet velocity yields the lower unburned carbon. Computer simulation also reveals that the higher inlet velocity gives the better mixing around the staging-air injection port, resulting in longer particle residence time, thus the lower unburned carbon.

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