A One Dimensional Model of Pulverized Coal Combustion in a Cylindrical Furnace and Its Experimental Validation

S. S. Dhumal and R. K.Saha
Department of Chemical Engineering, Indian Institute of Technology
Kharagpur 721302, India
Email: rks_iit@yahoo.co.uk
(Received on 18 Sep 2006, revised on 27 Mar 2007)

Abstract

The present paper describes a simplified one dimensional pulverized fuel flame model for predicting the performance of a flame in a cylindrical combustion chamber. The model does not take into account the variation between particle and gas temperature (which may be considerable), radial variation in flame properties, etc., but incorporates variation of particle size distribution, and evolution of volatiles and their combustion as distinct from char combustion. For the evolution of volatiles three different approaches are considered. In the first approach, the volatiles are assumed to be evolved and reacted rapidly with the present oxygen upto a certain distance from the entrance. Second approach is based on the single reaction kinetics for the evolution of the volatiles. To take into account the complexity of the devolatilisation phenomenon multiple reaction models is used in the third approach. Effects of various factors like particle size fractions, coal char reaction parameters and mechanism factor on the flame properties are evaluated. The predicted flame temperature profiles are then compared with the experimentally measured flame temperature profile. The comparison has been found to be satisfactory using multiple reaction models for the devolatilisation of coal.

Nomenclature

A	frequency factor of surface reaction rate (g/cm^2 s atm)
E	activation energy of reaction for char combustion (cal/mole)
E_v	activation energy of reaction for devolatilisation (cal/mole)
E_{v0}	mean activation energy for devolatilisation (cal/mole)
$f(E_v)$	distribution function for devolatilisation activation energy (mol/cal)
k_r	devolatilisation reaction rate constant ((volatile conc.)$^{n-1}$ s^{-1})
k_{r0}	frequency factor for devolatilisation ((volatile conc.)$^{n-1}$ s^{-1})
n	order of devolatilisation reaction
$p_g(U)$	partial pressure of oxygen in free stream when fraction of residual char unburnt is U (atm)
p_o	partial pressure of oxygen in fresh combustion air (atm)
R	gas constant (cal/mol K)
s	distance from burner (cm)
s_f	distance to complete evolution of volatiles (cm)
t	time (s)
T	temperature in the flame (K)
U	fraction of initial fixed carbon remaining unburnt
V	fraction of volatiles loss from coal up to time t

V^*	effective volatile content of coal
σ_v	standard deviation in activation energy distribution (cal / mol)
Φ	combustion mechanism factor

Introduction

Pulverized coal, as is introduced into a hot combustor usually leads to evolution of volatile matters (comprising moisture, CO, CO_2, hydrocarbons, tar vapours, etc.) followed by combustion of volatiles and char. The burning of volatiles may contribute as much as 30 – 40 % of the total heating value of coal. Therefore, they help in the process of ignition of coal char, so as to stabilize the formation of a pulverized fuel flame. The process is extremely complex and all the parameters cannot be incorporated into the modeling of a pulverized fuel flame. A simplified one-dimensional model of pulverized coal flame usually helps to qualitatively predict the flame performance. Though, a large volume of literature exists on modeling of pulverized coal flame; experimental data on lab scale furnaces using Indian coals are very rare. Without obtaining a detailed database on combustion characteristics of Indian coal in a laboratory scale test furnace and comparing them with theoretically predicted flame performance, it will be difficult to identify the design constraints and modification to be adopted for large-scale pulverized fuel fired boilers that are operating in India.

This paper describes a mathematical model that is designed to simulate the combustion and heat transfer processes in an experimental pulverized coal combustion chamber. The combustion chamber consisted of a horizontal steel tube, water cooled throughout its length. Primary air and pulverized coal were fired axially through a primary nozzle, and secondary air is introduced in an annulus concentric with primary nozzle. Heat transfer to wall was believed to occur predominantly by radiation only by assuming internally adiabatic process. Though, in a real pulverized fuel flame radial variation of flame properties including temperature variation exists, for simplicity in formulation and calculation scheme, a one dimensional flame is considered. In addition, devolatilisation schemes considering both a single reaction as well as a multiple reaction scheme are also incorporated in order to take care of the initial flame formation and ignition process in a proper way. Finally, the predicted flame temperature profile is compared with experimental flame temperature profile.

Model

The purpose of the model is to estimate, for all distances down the reactor (furnace), of the burn out (fraction of carbon remaining unburnt, U), the oxygen partial pressure and the radiation to the walls and the temperature. These quantities are to be calculated for various numerical values of the factors influencing them, in order to establish the sensitivity of the quantities to these factors.

Assumptions

The assumed flow pattern is illustrated in Fig. 1. Details of the assumptions are described below:

i) The flame expands conically to the point of impingement on the walls, beyond which it fills the whole cross-section.

ii) The rate of entrainment of secondary air per unit length of the chamber into the flame is constant up to the point where all the secondary air has been entrained. A re-circulation eddy occupies the space outside the flame between the burner and the point of impingement. The core of this eddy i.e. the point where the fluid is neither being entrained by, nor withdrawn from the jet is assumed to be at a distance from the burner, which is three quarters of the distance from the burner to the point of impingement.

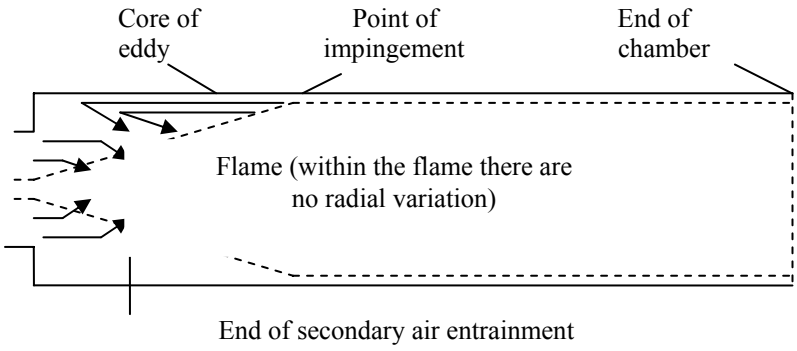

Fig.1 The assumed flow pattern

iii) The rate of entrainment of re-circulated fluid per unit length and the rate of extraction of fluid per unit length from the flame into the eddy are both assumed to be constant throughout the section in which these processes are occurring.

iv) Combustion in the re-circulation eddy is assumed to be complete before the fluid re-enters the flame.

v) Radial mixing within the flame is assumed to be rapid that there is no radial variation of concentration, temperature or velocity and there is no longitudinal mixing.

vi) The particle move at the same velocity as the gas stream.

vii) Particle emissivity is assumed to be constant.

viii) The absorption coefficient of the gas is assumed to be constant.

ix) Radiation from soot and ash is ignored.
x) Gas and particle temperatures are assumed to be equal.

xi) The specific heat of the suspension is assumed to be constant.

xii) The fuel is assumed to be polysize suspension of coal particles.

xiii) The particles are assumed to burn from the outside maintaining a constant density.

The flame is divided into two parts: one up to the point of impingement and beyond that. Based on mass balance of char and oxygen in these zones the flow rates are evaluated and then based on char reaction model and mass transfer process of diffusing oxygen to the char surface the extent of char combustion, the heat release rate, etc. are evaluated. Finally, an energy balance is performed based on internal adiabatic process and the temperature profile and the amount of char remaining unburnt at different stage of the flame are obtained. The details of the model have been documented earlier [1-3]. The modification carried out in the study, namely, the incorporation of different version of devolatilisation model is presented here. The calculation scheme and also the flow chart adopted for the calculation scheme are presented here.

Coal Combustion Model

Pulverized coal, as introduced into the furnace, is heated rapidly by radiation from the flame as well as from the hot combustion chamber and releases its volatiles. These are subsequently burnt into CO_2 and H_2O vapor releasing a substantial portion of heat of combustion of original coal and, thereby, initiating the process of ignition of coal char and sustaining it further. The amount of volatiles released, apart from the

type of coal, depends on the rate of heating and the temperature at which the heating process occurs and it may be much more than the proximate volatile obtained in the laboratory. A large number of pyrolysis model, based on single reaction scheme as well as multiple reaction scheme have been reported in the literature [4-5]. Three different schemes are being tried over here. Effects of these models on the flame performance parameters are presented.

Char combustion model

The details of char reaction model adopted here has been discussed in the literature (4,5). Oxygen diffuses to the surface of the particle and reaction to the formation of CO /CO_2 occurs only at the surface of the particle. The particles burn by shrinking sphere mode and the reaction is of first order. The diffusional resistance of oxygen to the particle surface depends on whether CO or CO_2 forms at the particle surface, i.e the mechanism factor. When CO_2 forms at the particle surface, the mechanism factor is one, while it is two when CO is formed. The oxygen consumption rate at the particle surface (q) when surface reaction rate is controlling is given by:

$$q = K_s p_{s,} \tag{1}$$

where, K_s is the surface reaction rate constant and is equal to A. e^{-E/RT_s}.

E= activation energy of reaction of coal char with oxygen and A = Arrehenius rate constant. The values of A and E depends on the nature of coal char used and may vary drastically from one coal to the other.

Constant volatiles evolution rate model

It is assumed that the evolution of volatiles is a very fast process, which takes place before the char combustion [4]. So therefore, the temperature after the inlet increases suddenly to a high value, which is not realistic. The constant rate of evolution of volatiles introduced by D. W. Gill [4] with respect to distance from burner:

$$V = V^* s / s_f \tag{2}$$

where, V is the weight of the volatile matter that has been evolved at distance s, and s_f is the distance to complete evolution. The value of s_f is calculated from the rate of disappearance of film thickness around the spherical particle.

Single reaction model (SRM)

The complex decomposition and transport phenomena involved in coal pyrolysis are not yet amenable to exact description. In this model, the overall process of pyrolysis of coal is approximated as a first order decomposition [5] occurring uniformly throughout the particle. So, the volatile and char combustion takes place simultaneously in the furnace.

$$\frac{dV}{dt} = k_r (V^* - V) \tag{3}$$

The rate constant in the above equation correlated with the temperature by an Arrhenius expression:

$$k_r = k_{r0} \exp(-E_v / RT) \tag{4}$$

Multiple reaction models (MRM)

The pyrolysis of coal is a very complex phenomenon which is not possible to represent by single reaction. Pitt's recognized the problem of devolatilisation by treating pyrolysis process to consist of a large number of independent parallel rate processes. Pitt's proposed a multiple reaction models [5] for coal decomposition under the non-isothermal conditions by using four parameters (V^*, E_{v0} , σ_v, k_{r0}).

$$\frac{V^* - V}{V^*} = \frac{1}{\sigma_v (2\pi)^{1/2}} \int_0^{\infty} \exp[-k_{r0} (\int_0^t \exp(\frac{-E_v}{RT}) dt) - \frac{(E_v - E_{v0})^2}{2\sigma_v^{\ 2}}] dE_v \qquad (5)$$

Experimental Details

The line diagram of the experimental set-up is shown in Fig.2. The dotted line shown in the figure indicates the thermocouple connections to the data logger followed by PC for online data. The solid lines indicate the feed to the respective unit.

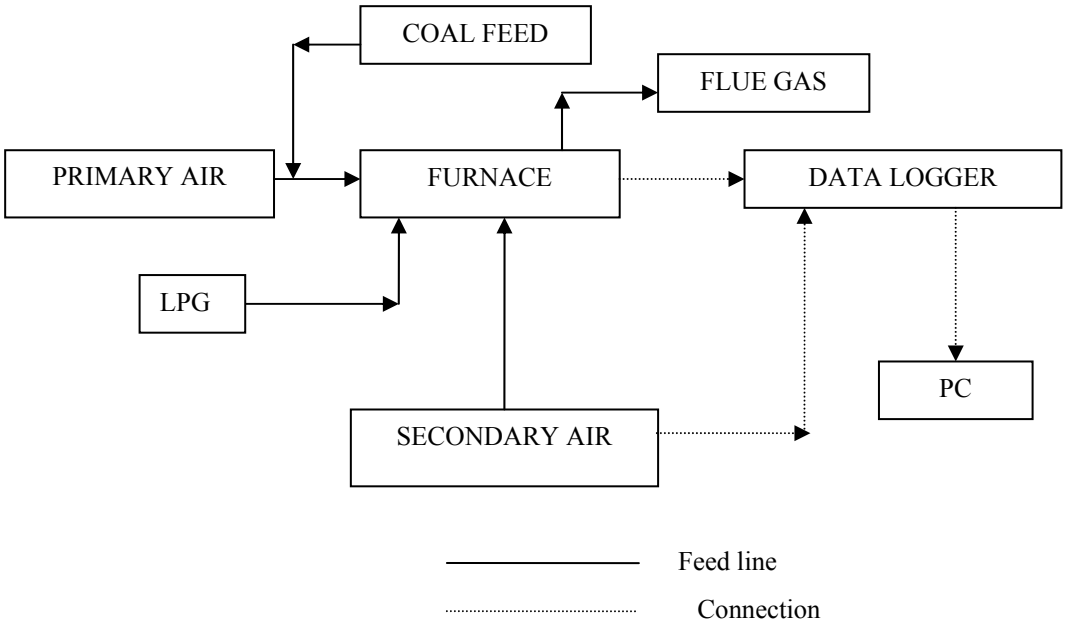

Fig. 2 Line diagram the experimental set-up

The furnace used for experimentation is having 275 cm length and 38 cm inside diameter. It is lined inside with 10 cm thick refractory bricks followed by 10 cm thick insulation of asbestoses rope to minimize the heat loss to the surrounding and provided with nine windows along the length for insertion of sampling probes. Opposite to each window, thermocouple is inserted into the furnace wall for measuring its temperature. At one end of the furnace, the pulverized coal burner is attached and at the other end, a recuperator for preheating the secondary air is installed. A 280 cm long muffle tube furnace is incorporated between the exit of secondary air from the recuperator and its entry into the burner, for preheating the secondary air up to 500^0C. The power input into the muffle furnace is regulated through three rheostats. The furnace is provided with four windows at the bottom for removal of the fly ash deposited during the experiments.

Results and Discussion

The model presented above and the given system of equations are to be solved to yield the variation with distance along the furnace of the fraction of carbon unburnt, the oxygen concentration, the flame temperature and radiation per unit length for each type of model. The flow diagram for the computation of the model is given in Fig. 3.

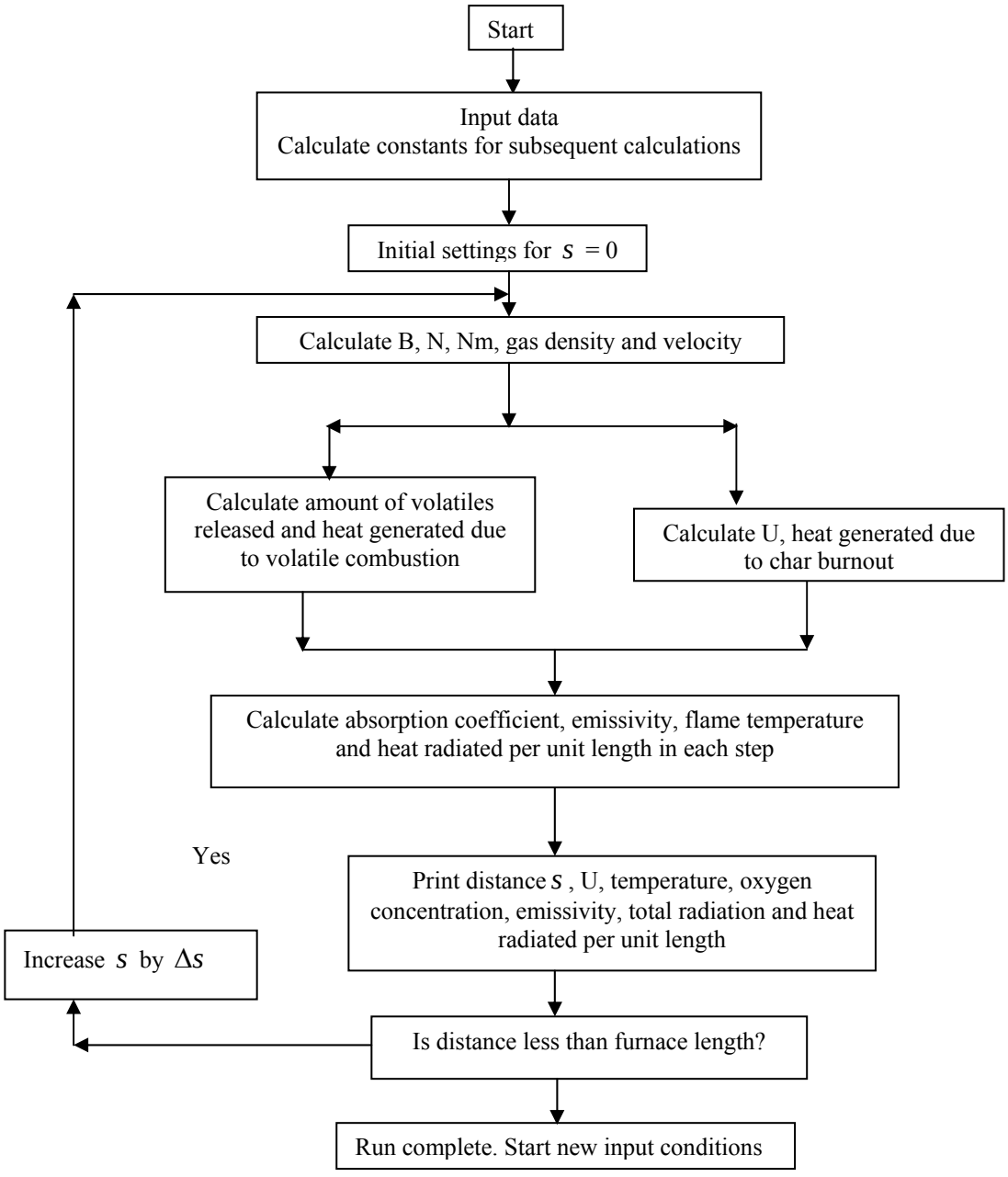

Fig. 3 Flow diagram for computation

The principle of the method of solution is to calculate the value of a variable at distance ($s + \Delta s$), from its value at time s and the rate of change of the variable at distance s. The method is typified by the expression:

$$y(s + \Delta s) = y(s) + y'(s)\Delta s \tag{6}$$

This is known as Euler's method. This method is used because it gives satisfactory results if the time interval is sufficiently short and it has advantage of flexibility and simplicity. A summary of data required for complete calculation and its values are given in Table 1 [1-4, 6].

Table 1 Parameter values

Parameter	Value	Parameter	Value
P	1 atm	R	1.98 cal/ mole K
$\overline{T}$	1400 K	L	275 cm
ρ_g at $\overline{T}$	0.252 x 10^{-3} g/cm^3	ρ_a	0.8 g/cm^3
$\overline{D}$ at $\overline{T}$	2.79 cm^2 /s	η_{fc}	0.202022
p_o	0.210 atm	m_p	4.53745
c_p	0.265 cal/g K	e	30%
Q	5200 cal/g	s_f	11.8282 cm
Q_v	8000 cal/g	s_c	83.3625 cm
$\in_p$	1.0	s_2	64.088475 cm
T_b	503 K	s_r	111.15 cm
T_r	1200 K	r_o	1.25 cm
T_w	940 K	r_f	19 cm
$N_{\max}$	1.2	A	24.5 g/cm^2.s.atm
B_o	3.0	E	18000 cal/mol
c	0.175085	k_{r0}	0.126337 s^{-1} (SRM)
Φ	2.0	E_v	6847.2704 cal /mol
$\overline{x}_o$	0.0061 cm	k_{r0}	5.656 x 10^{16} s^{-1} (MRM)
k_g	0.001 cm^{-1}	E_{v0}	70442.11 cal/mol
σ	1.36 x 10^{-12} cal/ cm^2 s K^4	σ_v	19303.859 cal/mol

The coal analysis, used for experimentation and calculation purpose is shown in Table 2. The devolatilization kinetics used in the present model was obtained earlier experimentally and has been published in earlier communication [6-7]. The amount of primary and secondary air used along with other specifications is shown in Table 3. The size distribution of char, shown in Table 4, is represented by 4, 7, 13 fractions. The char kinetic parameters, which are used in the program, are directly taken from the available

literature which can be determined from the experimental data on the gas analysis from the drop tube furnace.

Table 2 Analysis of Indian coal

Proximate analysis		Ultimate analysis	
Moisture	4 %	Carbon	71.0 %
Volatile Matter	25%	Hydrogen	3.9 %
Ash	11 %	Oxygen	11.35 %
Fixed Carbon	60 %	Nitrogen	1.75 %
		Sulphure	1.0 %

Table 3: Feed rate specifications

Coal feed rate	5.5 kg/h
Primary air rate	16.45 kg/h
Secondary air rate	49.3474 kg/h
Primary air temperature	305 K

Table 4 Representation of the size distribution of char

A: Representation by 13 fractions*

Fra. No. j	1	2	3	4	5	6	7	8	9	10	11	12	13
x_j (μm)	3	7	12	22	33	48	67	89	123	168	213	255	350
w_j	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.05	0.03	0.015	0.005

B: Representation by 7 fractions*

Fra. No. j	1	2	3	4	5	6	7
x_j (μm)	5	17	40	78	138	227	350
w_j	0.2	0.2	0.2	0.2	0.15	0.045	0.005

C: Representation by 4 fractions*

Fra. No. j	1	2	3	4
x_j (μm)	5	29	104	238
w_j	0.2	0.4	0.35	0.05

*All fractions having the equal weight mean diameter, which is equal to 61 μm .

Effect of Model Parameters

The multiple reaction models is used to study the effect of different parameters on the profiles of fraction of carbon unburnt, temperature etc.

Effect of number of fractions employed to represent the size distribution

The size distribution of char, shown in Table 4, is represented by 4, 7, 13 fractions. The effects of size distribution on the fraction of carbon unburnt are shown in Fig. 4. It is seen that results for 7 and 13 fractions are indistinguishable while result for 4 fractions differs slightly. But these differences are considered to be slightly small. It has been concluded that representation of a size distribution by either 7 or

13 fractions is adequate; but the distribution using 13 fractions has been used in the other computations reported here (the larger the number of fractions, the smoother is the distribution).

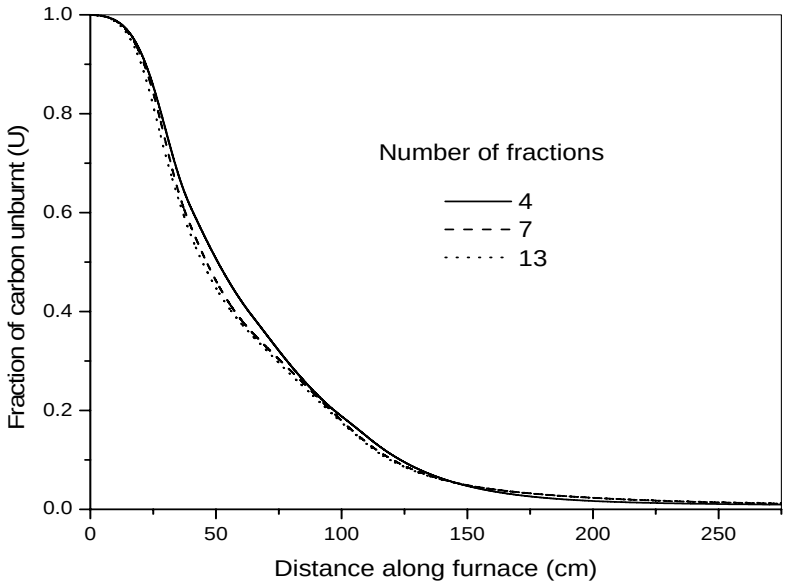

Fig. 4 Effect of number of fractions employed to represent the size distribution

Effect of reaction rate parameters for char combustion

For A = 1.65 g/cm^2.s.atm and A = 24.5 g/cm^2.s.atm, results are shown in Figs. 5 and 6.

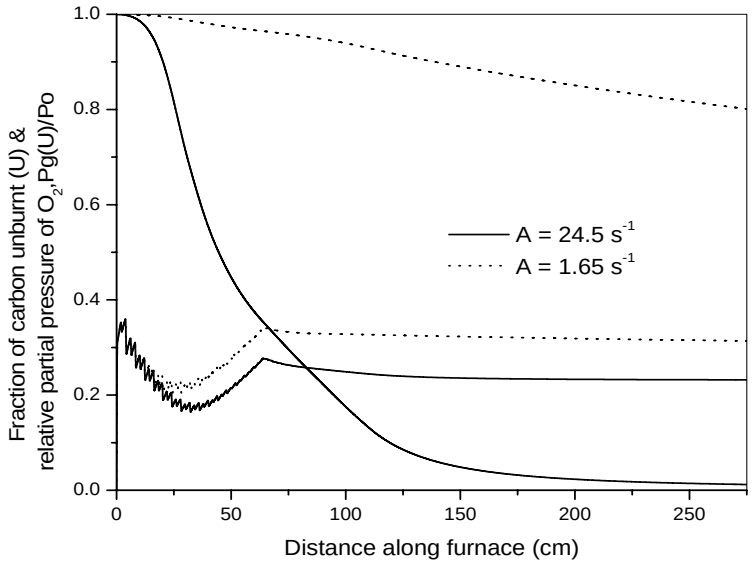

Fig. 5 Effect of frequency factor on U & Pg (U)/Po

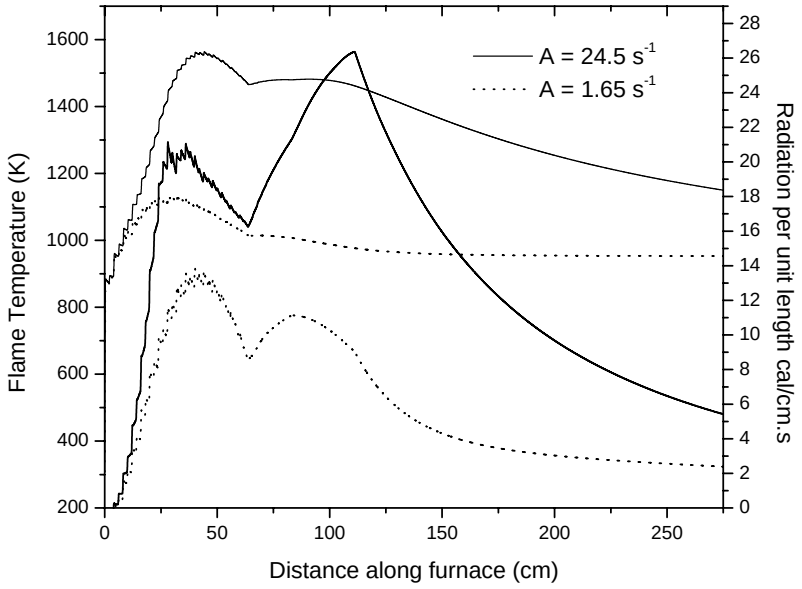

Fig. 6 Effect of frequency factor on flame temperature and radiation

With A = 1.65 g/cm^2.s.atm, the surface reaction rate is low as compared to the surface reaction rate at A = 24.5 g/cm^2.s.atm. With the low reaction rate a large proportion of the carbon remains unburnt, oxygen concentration is high and temperature drops to a low value.

Effect of mechanism factor (Φ)

The effect of the value of the mechanism factor Φ on the results, with the values of A = 24.5 g/cm^2.s.atm and E = 18000 cal /mol for char combustion, is shown in Figs.7 and 8.

The mechanism factor, which depends on whether the carbon is transported away from the particle surface as carbon monoxide (Φ =2) or carbon dioxide (Φ =1), determines the reaction rate under diffusion control. The effect on the rate of burn out is appreciable, as might be expected, where the rate of combustion is controlled to a large extent by diffusion. The effects on the oxygen concentration, flame temperature and the distribution of radiation are considered to be negligible.

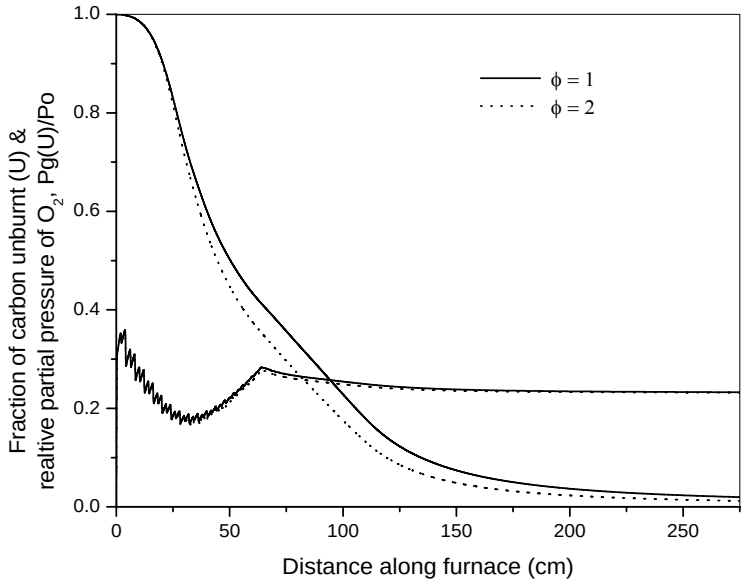

Fig. 7 Effect of mechanism factor (Φ)on U and Pg (U)/Po

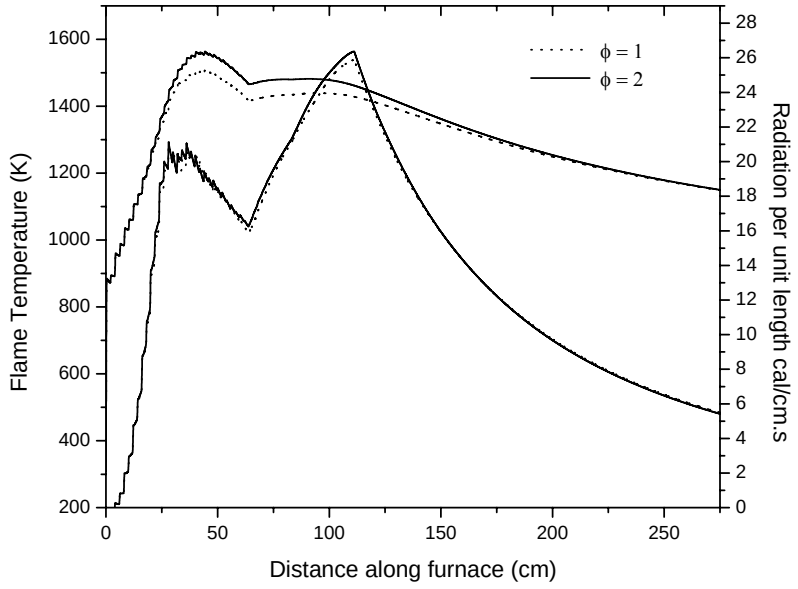

Fig. 8 Effect of mechanism factor (Φ) on flame temperature and radiation

Fig. 9 shows the dynamic response of the flame temperature. It shows that how temperature fluctuates after the suction pyrometer is inserted in the furnace with time.

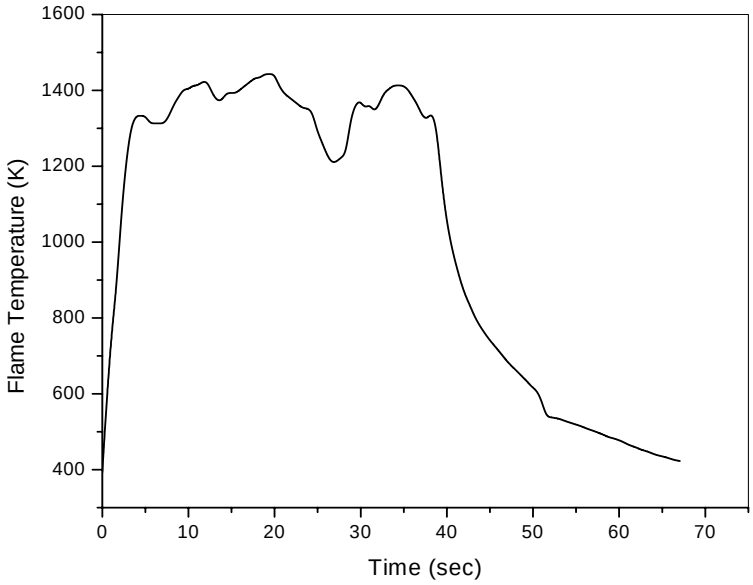

Fig. 9 Dynamic response of the flame temperature

The Fig.10 shows the radial temperature variation inside the furnace at different positions. The profile gets flattened as the distance from the burner increases. So the radial temperature profile is not axi-symmetric. This may happen due to the off centre location of the burner or the erosion of the burner because the furnace was designed and operated since last one decade.

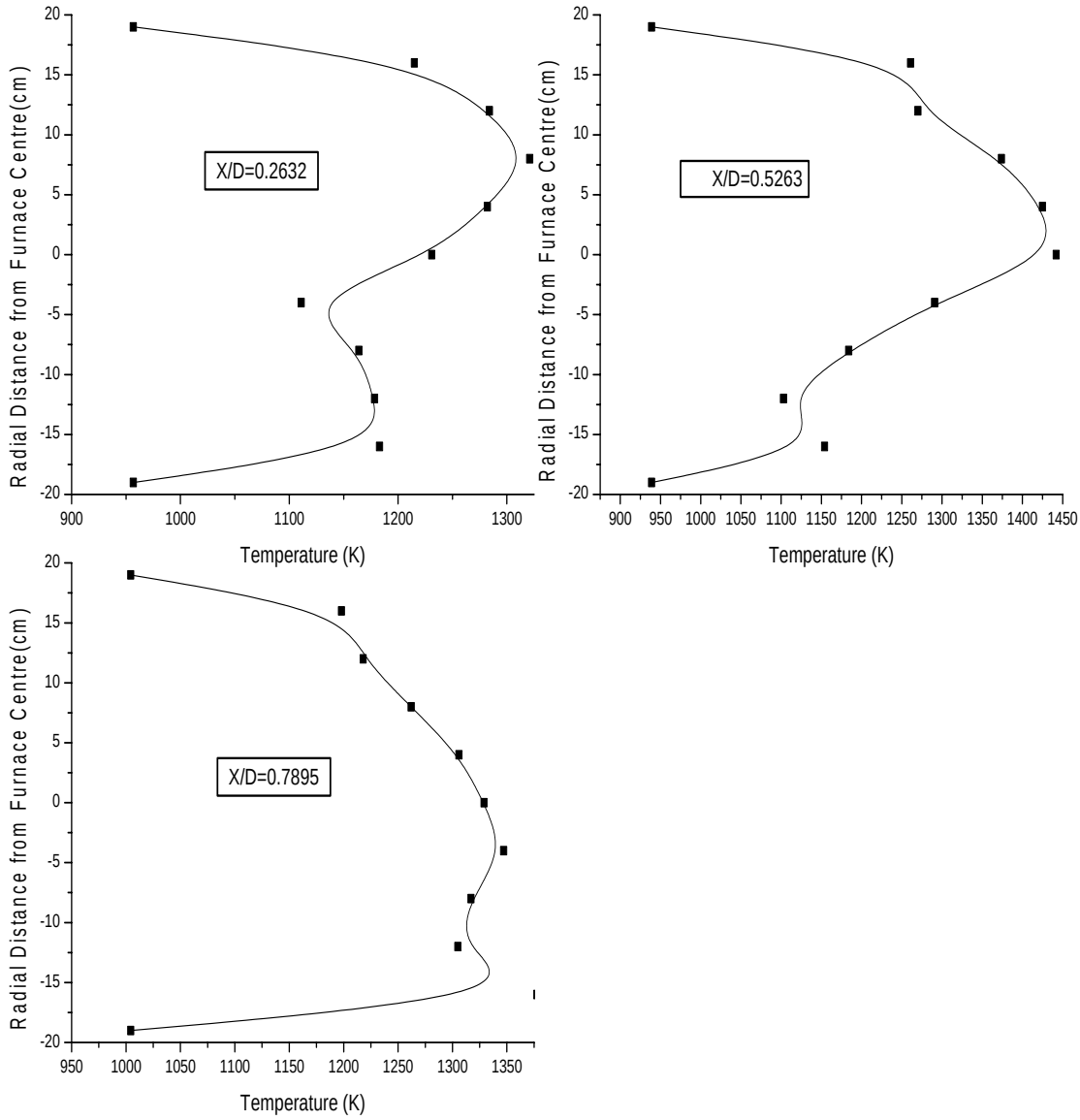

Fig. 10 Radial temperature profile in the furnace for different X/D ratio

The experimental results obtained from the laboratory scale furnace are being compared with the theoretical results of different models which are shown in the Fig. 11. Fig.12 shows the profiles of the fraction of carbon unburnt versus distance along the furnace for different models. The constant volatile evolution rate shows an unrealistic high temperature just after the burner which is not possible in reality. That's why the fraction of carbon unburnt profile shows a sudden decrease at the start.

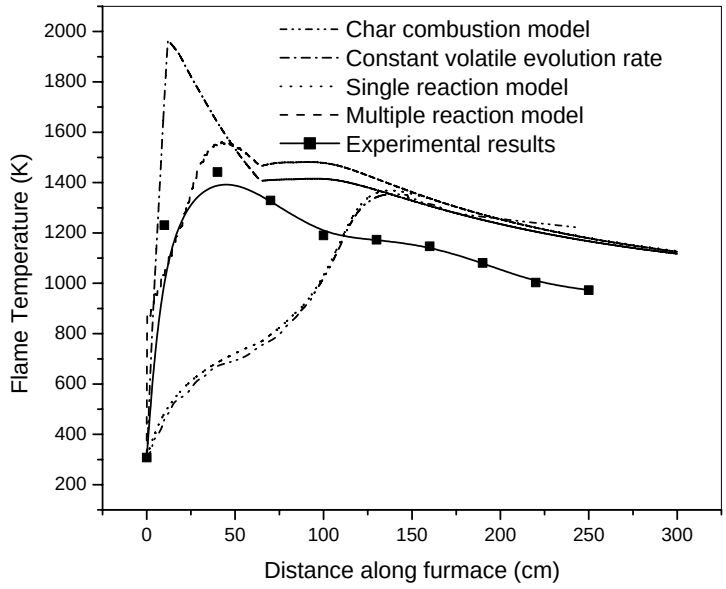

Fig. 11 Comparison of different models with the experimental results

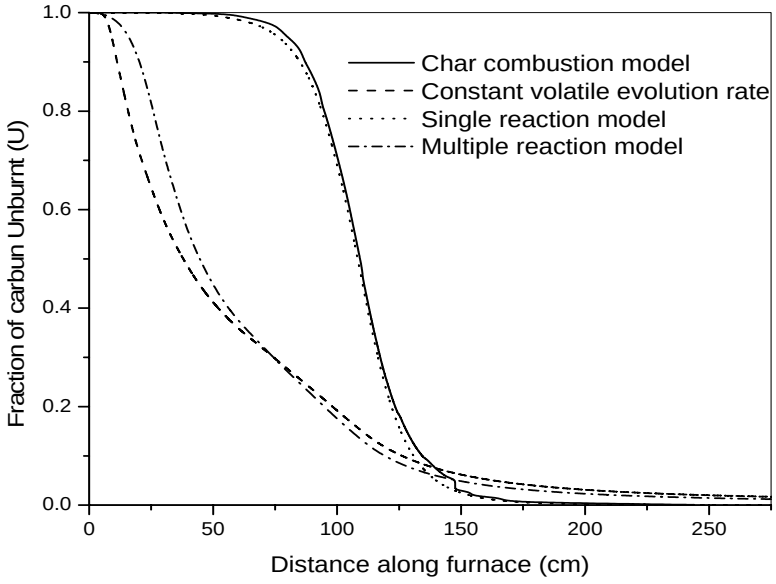

Fig. 12 Profiles of fraction of carbon unburnt for different models

The flame temperature profile obtained from the char combustion and the single reaction model are not satisfactory as compared to the experimental results. The reason behind this is, in the char combustion model the heat contribution from the volatiles is assumed to be negligible. In the single reaction model, the volatile evolution rate is very low. So there is no change in the profiles of the fraction of carbon unburnt at the starting length of the furnace for both models. Basically, to represent the pyrolysis behavior of the coal

the single reaction model is not satisfactory. This is the reason to present the multiple reaction models. The flame temperature profile obtained from the multiple reaction models follows the same path as like the experimental results. There is deviation in between the results of experimental and multiple reaction models after 40 cm length of the furnace. This is due to the heat loss to the surrounding via natural convection and/or radiation from the furnace surface which is not under control. But at the time of modeling the completely adiabatic system assumption is their. That's why multiple reaction models are the better representation of the coal pyrolysis.

Conclusion

After comparison of the axial temperature profile obtained from the lab scale furnace with the theoretical axial temperature profiles obtained from the different models, it is found that the multiple reaction models are in better agreement. The experimental profile follows the same path at the starting length of the furnace as like the theoretical results. After some distance it deviates downward, it may happen because of the heat loss from the flame to the surrounding.

The sensitivity of the results to the smoothness of the size distribution has been examined. It has been found that the results are insensitive to the smoothness of the size distribution provided that at least seven fractions are used to represent it. The results are found to be sensitive to the changes in the char reaction parameters. The mechanism factor won't affect that much the oxygen concentration, flame temperature and radiation but slightly affect the fraction unburnt profile.

The radial temperature profile obtained from the laboratory scale furnace flattens as the distance from the burner mouth increases. The radial profile is not an axi-symmetric. This may happen due to the off centre location of the burner or the erosion of the burner because the furnace was designed and operated since last one decade.

References

[1] S. S. Dhumal, "Kinetic study on pyrolysis of coal and modeling of pulverized fuel flame in cylindrical furnace", M. Tech. thesis, I. I. T. Kharagpur, India, 2004.

[2] M. A. Field, D. W. Gill, B. B. Morgan, and P. G. W. Hawksley, "Combustion of pulverized coal", BCURA, Vol. 257, pp. 455-523, 1966.

[3] M. A. Field, D. W. Gill, B. B. Morgan and P. G. W. Hawksley, "Combustion of pulverized coal", BCURA, Vol. 259-264, pp. 81-485, 1967.

[4] D. W. Gill, "Extension to a one dimensional mathematical model of a pulverized coal flame", BCURA Report No. 356, pp. 1-12, March 1969.

[5] M. A. Elliott, "Chemistry of coal utilization", Wiley, New York, pp. 727- 753, 1981.

[6] S. S. Dhumal and R. K. Saha, "Application of genetic algorithm for evaluation of kinetic parameters of coal pyrolysis", Journal of Energy & Environment, Vol. 5, pp. 112-124, 2006.

[7] R. K. Saha, "Studies on pyrolysis of coal", Journal of Institution of Engineers, India, Vol. 64, pp. 56-59, 1984.