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RESEARCH ARTICLE

Modeling Flame Propagation of Coal Char Particles in Heterogeneous Media

Mehdi Bidabadi[1], Moein Mohammadi[1*], Shafagh M. Bidokhti[1],
Alireza K. Poorfar[1], Saeedreza Zadsirjan[2], Massoud Shariati[1]

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Abstract

In the present research, combustion of a quiescent coal char particle cloud has been studied in the media with spatially discrete sources by means of numerical approach. A thermal model based on diffusion-controlled regime of coal char particles has been generated in order to estimate the characteristics of flame propagation in heterogeneous media. The model uses discrete heat sources to analyze dust combustion of particles with the diameter of 50 μm. Oxygen and Nitrogen have been considered as the main oxidizer and the inert gas, respectively. Flame propagation speed in various dust and oxygen concentrations has been studied. Flame speed as a function of particle size has been investigated and comparison between cases with and without consideration of radiation effect has been made. Furthermore, minimum ignition energy as a function of dust concentration for different particle sizes has been studied. Results show a reasonable compatibility with the existing experimental data.

Keywords

Coal char particles, Discrete Combustion, Thermal model, Flame Speed, Minimum Ignition Energy, Radiation

1 Introduction

Combustion of char particles is related to pulverized coal combustion, burning of heavy fuel oil, particulate emission through soot oxidation, and propulsion, due to its high energy density. Consequently, extensive studies have been conducted, as summarized in several comprehensive reviews [1-5]. Because of its low price and ease of use, coal will continue to be one of the main energy sources. Hence, combustion of coal attracted a considerable amount of theoretical and experimental investigations.

On the other hand, dust explosion has been a recognized threat to humans and industries for the last 150 years [6-11]. The occurrence of three fatal combustible dust explosions within one year in 2003 prompted the U.S. Chemical Safety and Hazard Investigation Board (CSB) to commence a broader study on the extent, nature and prevention of combustible dust fire and explosion hazards. Methane and coal dust explosions are the most feared hazards in the coal industry worldwide [12]. The large majority of these explosions originates from or occurs around sealed mine areas [13]. Such events have prompted industries to study dust combustion characteristics to seek the means to reduce the effects of dust combustion.

Thus, a precise knowledge of dust explosion's hazards is essential to estimate the consequences of a dust explosion and to select the adequate methods of protection such as venting (e.g., explosion relief vents) and suppression systems.

Propagating diffusion fronts in reactive, heterogeneous media consisting of two spatially separated phases are common in many fields such as chemical kinetics, combustion, biology, etc. [14]. In addition, fire dynamics and modelling of fire spreading are some of important examples in heterogeneous media.

Goroshin et al. [15] studied the effects of the discrete nature of heat sources on flame propagation in particulate suspensions. They illustrated the effect of the discrete nature of the heat sources on flame propagation by comparing flame speeds calculated both from continuous and discrete models in lean Aluminium and Zirconium particle-gas suspensions. It is reported in their work that the discrete flame model predicts lower flame speeds and a weaker dependence of the speed on Oxygen concentration. Tang et al. [16] investigated the effect of discreteness on

[1] Combustion Research Laboratory, School of Mechanical Engineering,
Iran University of Science and Technology (IUST)
Narmak, 16846-13114 Tehran, Iran

[2] Department of Aerospace Engineering,
Amirkabir University of Technology (Tehran Polytechnic),
424 Hafez Ave, Tehran, Iran

[*] Corresponding author, e-mail: moeinmohammadi@mecheng.iust.ac.ir

heterogeneous flames and propagation limits in regular and random particles. Mendez et al. [17], also, studied the speed of reaction-diffusion fronts in spatially heterogeneous media.

Because of coal reaction with oxygen in the air, which is an exothermic reaction even in ambient condition and probability of its thermal runaway, combustion of coal is an important safety issue in mines [18]. To prevent disasters in coal mines and also to improve fundamental understanding of the phenomenon, researches on the combustion of coal dust cloud have been conducted for a long time. Also pulverized coal combustion is mainly used as an energy source in practical use. The pulverization of coal into fine particles are made to increase the specific surface area to enhance the rate of heat and mass transfer between the coal particles and surrounding hot gases. This, on the other hand, will increase the importance of the continuity or discreteness of the system.

Regarding flame stability, flame propagation behaviour in coal dust clouds seems to be one of the important properties for predicting the performance of a new burner [19]. Most of the experimental studies mainly deal with the influence of coal composition on combustion of coal and different stages of coal combustion [20]. Numerical studies, on the other hand, deal with the modelling of different stages of combustion process.

Bermudez et al. [21] investigated a mathematical model for combustion of coal particles with a simplified kinetic model. Their model included the change in diameter of the particles. Kun Li et al. [22], also, studied particle combustion by considering both volatile and carbon reactions. In their model, they assumed that flame moves from off the particle to the surface of the particle after a homogenous burning process. Most of the models for coal combustion neglect the discrete nature of this process and deal with it as a continuous phenomenon.

The coal particle contains a fix carbon part, also known as char, and volatiles (a mixture of light gases and tars). Concisely, the combustion of initial coal particle consists of four main parts, which are vaporization, devolatilisation, burning of volatiles and combustion of the remaining char. The latter is much slower than devolatilisation and burning of the volatiles and, therefore, determines the burnout time of the coal particles. The combustion of the remaining char involves an interaction of heterogeneous and homogeneous reactions and transport limitations.

In the present study, the effects of char particle size and dust concentration on flame propagation of micron- sized dust particles in media with spatially discrete sources are studied numerically. A thermal model based on discrete heat sources viewpoint has been utilized. Flame propagation speed as a function of dust concentration and particle size has been investigated. In addition, the minimum ignition energy as a function of dust concentration for different particle diameters has been studied. It should also be noted that available experimental results are in poor agreement with each other, apparently, due to different test conditions and differences in internal structure of examined particles.

2 Thermal Model

The mechanism of the combustion of dust clouds is a very complex process. The difficulty in their study is due to various processes such as heating, evaporation, mixing with oxidizer, ignition, burning and quenching of particles in the dust cloud. In the study of flame propagation in dust clouds, particle size and dust concentration play very important roles. In addition, the interaction between the particles in the mixture always makes the dust combustion an unstable process. Heat transfer is the dominant phenomenon in the process of flame propagation in dust clouds.

A thermal model established on heterogeneous combustion in three-dimensional space, which relies under the following assumptions, has been generated:

1. Burning particles in air are assumed to be spherical and the flame diameter remains constant and is equal to the particle diameter.
2. The ignition is supposed to occur in a layer of particles simultaneously so the flame propagation will be planar type.
3. The burning process is quasi-steady.
4. The physical and thermal properties of particles and the media, such as thermal conductivity, specific heat and density are assumed constant during the burning process.
5. Gravitational forces are neglected to overcome the buoyancy effects.
6. There is an equal and constant space between the particles distributed in the dust cloud.
7. A constant rate of energy release is considered during the combustion of a single particle.

Levendis et al. [23] presented an equation for burning time of a single micron-sized char particle. The combustion mode of micron-sized char particles is a diffusion-controlled regime. In addition, char undergoes a heterogeneous combustion in oxygen. The burning time of char particles in diffusion-controlled regime can be obtained from the following equation [23]:

$$\boldsymbol{t}_{b_{diff}} = \frac{\rho_p \left(d_{p,i}^2 - d_{p,f}^2\right) R T_m}{56 D_{O_{2,\infty}} \ln\left(1 + 0,75 Y_{O_{2,\infty}}\right)} \tag{1}$$

Where $t_{b,diff}$ is the burning time of char particle in diffusion-controlled regime, ρ_p is the apparent density of coal particle, $d_{p,i}$ and $d_{p,f}$ are the initial and final diameters of the particle, respectively. R is the ideal gas constant, T_m is the mean temperature in the film, $D_{O2,\infty}$ is the mass diffusivity of oxygen into the air, and $Y_{O2,\infty}$ is the mass fraction of oxygen in the ambient gas far from the particle surface.

2.1 Governing Equations

2.1.1 Conduction Heat Transfer

As the minimum amount of energy is provided to the dust cloud by the ignition system, the temperature of some particles is increased to the ignition temperature. When these particles start to combust, they play the role of a heat source in the dust cloud system and it results in a temperature rise in the surrounding region. The temperature rise in other particles is determined by summing the thermal effects from the burned and burning particles. When the temperature reaches a certain threshold, the combustion will pass to the other particles, as shown in Fig. 1.

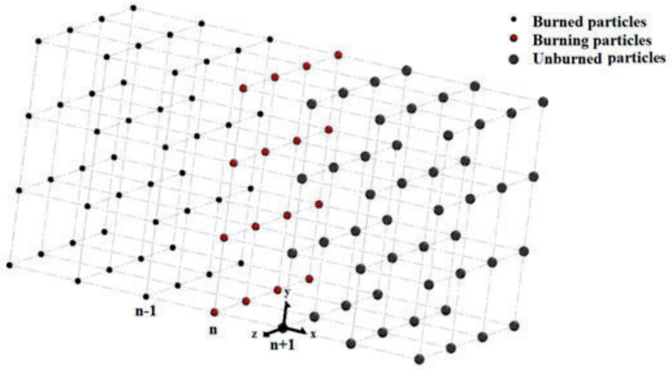

Fig. 1 The spatial distribution of particles in dust cloud: Layer n−1 (burned particles), layer n (burning particles), and layer n+1 (unburned particles)

The increase in the temperature of particles in the preheated zone due to conduction heat transfer only is stated based on the superposition principle. In order to model the single-particle combustion and the time-place temperature distribution of its domain, the energy equation in spherical coordinates is used:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T_a(r,t)}{\partial r}\right)=\frac{1}{\alpha}\frac{\partial T_a(r,t)}{\partial t} \tag{2}$$

Where $T_a(r,t)$ is $T(r,t)-T_\infty$, and T_∞ is the ambient temperature. The boundary and initial conditions of the above equation are:

$$\left\{\begin{array}{l} k_pA_p\frac{\partial}{\partial r}T_a(r,t)=\dot{q}\times Heaviside(\tau-t)\quad at\quad r=r_p \\ T_a(\infty,t)=0 \\ T_a(r,0)=0 \end{array}\right\} \tag{3}$$

Where k_p and A_p are thermal conductivity and surface- area of the particle, respectively. q is the rate of heat release of a single particle which is released from its surface while burning, and defined as below [24]:

$$\dot{q}=Ak_p(T_f-T_\infty)r_p^{-1} \tag{4}$$

The space-time temperature distribution of particles through the whole domain has been obtained as stated below:

$$T_a(r,t)=\left(T_f-T_\infty\right)\frac{r_p}{r}\left[erf\left(\sqrt{\frac{(r-r_p)^2}{4\alpha t}}\right)-Heaviside(t-\tau)erfc\left(\sqrt{\frac{(r-r_p)^2}{4\alpha(t-\tau)}}\right)\right] \tag{5}$$

$$T_s=\sum_i\sum_j\sum_k T_a(i,j,k)(r_{i,j,k},t_{ig,i}) \tag{6}$$

T_a is the space-time distribution of temperature of single burning particle surroundings and beyond, and T_s is the total effect of particles during and after combustion which indicates the temperature of the media surrounding a particle in the preheated zone. T_∞ =300 K and T_f= 3700 K are the considered values [15]. i, j and k denote the number of layers from the specific particle to any particle along each axis. Consequently, the space between these particles is presented by:

$$r_{i,j,k}=L\sqrt{i^2+j^2+k^2} \tag{7}$$

Where L is the space between two adjacent layers which is defined by the equation below [25]:

$$L=\left(\pi d_p^3\rho_p/6C_d\right)^{1/3} \tag{8}$$

Where ρ_p is the particle density, C_d is the dust cloud concentration, and d_p is the particle diameter. The flame propagation speed is defined as the ratio of the space between two adjacent layers to the difference of their ignition times [26]. As mentioned earlier, since micron- sized particles are being dealt with, the formulation presented by Glassman and Yetter [27] is utilized here. Fig. 1 shows the spatial distribution of particles in dust cloud. The ignition time of a single particle in a layer can be the representative of the ignition time of that layer. The particle is assumed to be positioned at the origin of the local coordinate system.

2.1.2 Radiation Heat Transfer

The propagation of flame in the cloud particles is performed by the conduction and radiation heat transfer mechanisms.The temperature of the particle is determined based on the amount of energy transferred and the heat capacity of the particle. For this purpose, it is necessary to solve Eq. (9), the energy equation of a particle:

$$Q_{rad}+Q_c=\rho c_pV\frac{dT_p}{dt} \tag{9}$$

C_p is the average heat capacity which is taken a constant value at a given range of temperature between the ignition temperature and adiabatic flame temperature. Q_{rad} is the radiation heat transfer and Q_c is the conduction heat transfer which is obtained by the below equation [24]:

$$Q_c=HA_p(T_s-T_p) \tag{10}$$

T_s is the temperature of the gas surrounding the particle which is calculated from the previous section and T_p is the temperature of the particle, A_p is the surface-area of the particle and

H is the convective heat transfer coefficient. Since the particle is considered spherical so [24]:

$$Nu = \frac{Hd_p}{\lambda} \cong 2 \tag{11}$$

Where Nu is the Nusselt number and λ is the heat conductivity coefficient. Using above equation and substituting in equation (10), we have:

$$Q_c = \frac{2\lambda A_p}{d_p}(T_s - T_p) \tag{12}$$

Radiation in a dust cloud mixture is considered to be as the radiation in a gray two-phase environment [28]. This environment incorporates the coefficients of emission, absorption and scattering of thermal radiation intensity.

$$\frac{dl}{dx} = +K_a I + K_s I - K_a I_b - \frac{K_s}{4\pi}\int_{4\pi} I(\Omega)P(\theta,\Phi)d\Omega \tag{13}$$

The terms on the right side of Eq. (13) represent the radiation intensities resulting from absorption, scattering, emission, and also the radiation intensity due to the scattering of the other particles respectively. K_s, K_a and I are the scattering, absorption coefficients and radiation intensity, respectively. $P(\Theta, \Phi)$ is the phase function for scattering [29], and I_b is the black body emission power, which depends on the local temperature of particles. All particles in this two-phase environment are assumed to have a spherical shape and uniform size. They all have positive values, and I decrease as x (distance variable) increases. In a two-phase mixture with uniform particles, K_a and K_s are obtained through the below equations [30];

$$K_a = \frac{\pi d_p^2 . n_s}{4} Q_{abs} \tag{14}$$

$$K_s = \frac{\pi d_p^2 . n_s}{4} Q_{Sca} \tag{15}$$

Where Q_{abs} and Q_{sca} are the absorption and scattering efficiencies and d_p and n_s are the particle diameter and the number of particles per unit volume. The absorption and scattering efficiencies of these spheres can be considered as following. In case the particles act as perfect reflective scattering spheres:

$$\begin{Bmatrix} Q_{abs} = \varepsilon \\ Q_{sca} = 1 - \varepsilon \end{Bmatrix} \tag{16}$$

Where ε is the solid particle's emission capability.

The equations are difficult to solve because of the integral term on the right hand side of the Eq. (13). The integral term represents multiple scattering. If it is assumed that the multiple scattering is negligible and the intermediary matter propagates throughout the pre-heating process, only the absorbed energy will remain which is then converted to the internal energy; therefore, the radiation in the pre-heating zone is expressed as following [28]:

$$\begin{gathered} Q_r = K_a I_f \exp(-K_t x) \\ \left\{ K_t = K_a + K_s \qquad I_f = \frac{K_a}{K_t} I_{bp} \right\} \end{gathered} \tag{17}$$

Where I_f is the intensity of radiation, induced from the flame front into the pre-heating and vaporization zones. Also x, σ and T_f are distance variable, the Stefan- Boltzmann constant, and flame temperature, respectively.

2.1.3 Flame Radiation Model

The heat transfer via radiation to a single particle should be obtained before being generalized to the discrete model. The Q_r calculated in the previous section is the amount of heat radiated to pre-heating zone from the burning particles of the dust cloud, and it can be used to estimate the amount of radiation per unit area. This means that, this is the amount of energy that all the existing particles in a layer with an area of unity receive in the pre-heating zone. In a unit area, the number of particles in a layer is determined by the following expression:

$$n_L = L^{-2} \tag{18}$$

Thus, the amount of radiation heat transferred via radiation from the combustion zone to a particle in the pre-heating zone is obtained through dividing Q_{abs} by n_L;

$$q_r = Q_r / n_L \tag{19}$$

Using equations (16), (17) and substituting in equation (19) we have [31]:

$$q_r = \frac{d_p^2}{4L}\varepsilon^2 \sigma T_f^{\,4} \exp\left(\frac{-\pi d_p^2}{4L^3}x\right) \tag{20}$$

As stated in the previous sections it is assumed that radiation is only emitted from the burning layers. The second layer is ignited after the ignition of the first layer, which causes its particles temperature reach the ignition temperature of fuel and the subsequent layers are ignited in the same way. Therefore, each layer has a unique ignition time. As a result, the radiated energy from a burning layer depends on its time of combustion.

The sum of energy emitted from the burning layers determines the total energy transferred to a particle in the pre-heating zone. Assuming the number of burning layers to be n_b, the following expression can determine the total radiation heat transferred to a particle in the pre-heating zone:

$$Q_{rad} = \sum_{l}^{n_b} q_r(x,t) \tag{21}$$

By substituting Q_{rad} and Q_c in the Eq. (9) we have:

$$Q_{rad} + \frac{2kA_p}{d_p}(T_S - T_p) = \rho c_p V \frac{dT_p}{dt} \tag{22}$$

The above equation covers the effect of radiation and conduction mechanisms in increasing the temperature of the target particle.

3 Results and Discussion

A MATLAB code has been generated to compute the burning velocity and ignition time of each layer after the discharge of the energy from the ignition system. The logic and algorithm of the program is shown in Fig 2.

In fact the theoretical model is based on analytical approach. How ever, to obtain the final results of the governing equations, a computational method has been utilized.

In the considered algorithm, following the release of energy, at first, the temperature of the first layer due to the ignition system at the considered location is calculated. As temperature of the particles of the first layer reaches the ignition temperature, it is registered as the first layer ignition time and the program continues to find the ignition times of the other layers.

Further than the first layer (n > 1), preheating of other layers is affected by both burning of the previous layers and the ignition system. Therefore, when temperature of a layer reaches the ignition temperature, the corresponding time is registered as the ignition time of that layer. Flame propagation speed can be calculated via dividing the distance between two adjacent layers *L* by the difference between ignition times of these two layers. The rise of particle's temperature will be a function of thermal diffusivity α , if it is assumed that conduction is the only mechanism of flame propagation. The higher this value, the sooner the adjacent layers reach the ignition temperature and the flame propagation speed increases.

Regarding the radiation mechanism, any factor which causes a rise in the number of simultaneously burning layers, will contribute to the increase of radiation intensity. We assume that radiation heat transfer issues only from a burning layer, and it stops when that layer burns out. Therefore, the radiation intensity is higher when there is a lesser time difference between the ignitions of adjacent layers which means that more layers are burning at the same time. If the radiation intensity increases, the influence of radiation heat transfer becomes more significant than that of conduction. As long as the radiation intensity has not reached its critical value, the layers in the preheated zone ignite one after the other. At the beginning the difference between the ignitions times of adjacent layers, $t_{ig}(\mathrm{n}+1) - t_{ig}(\mathrm{n})$, which is proportional to flame advancement speed, varies for both adjacent layers. However, as the flame propagates, this propagation speed value will become stable.

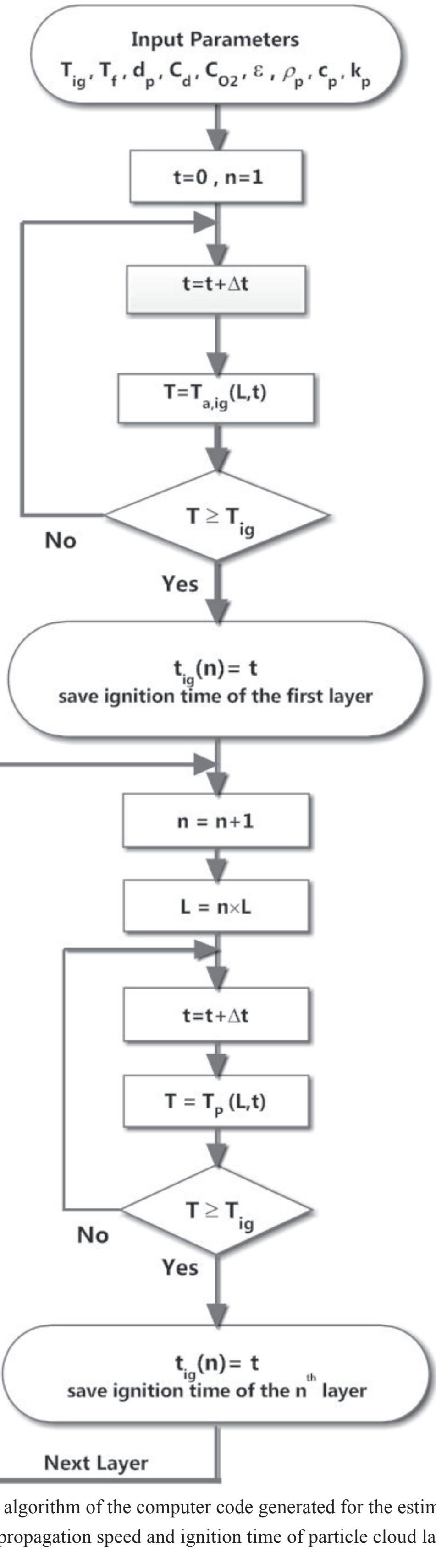

Fig. 2 The algorithm of the computer code generated for the estimation of flame propagation speed and ignition time of particle cloud layers

Figure 3 illustrates the comparison of the theoretical flame propagation speed with experimental data obtained in [19] in terms of dust concentration. With the increase of dust concentration, flame propagation speed tends to increase. When

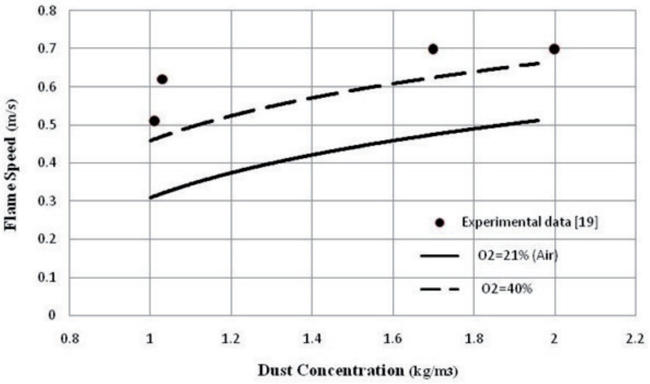

Fig. 3 Flame propagation speed as a function of dust concentration for 50 µm particles

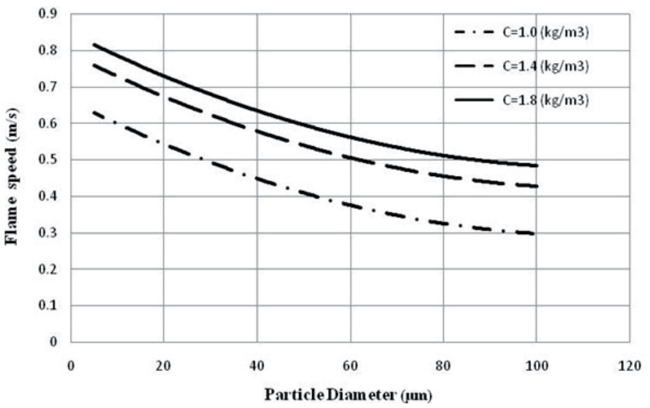

Fig. 4 Flame speed as a function of particle size in different values of dust concentration

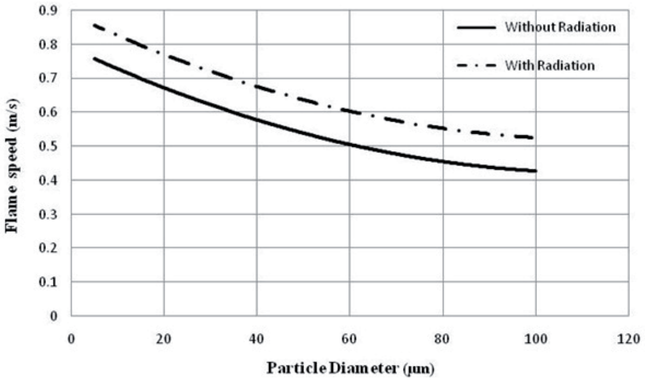

Fig. 5 Flame speed as a function of particle size with and without the consideration of radiation effect

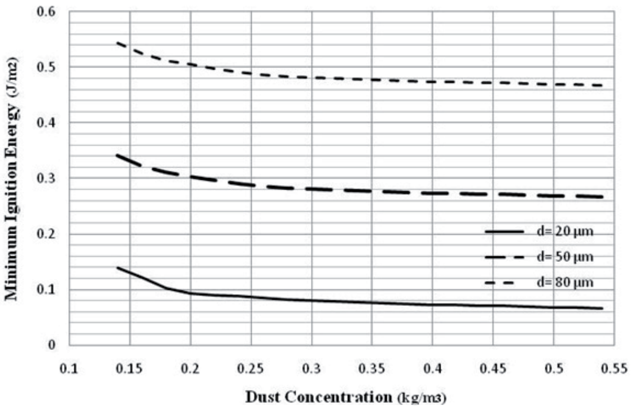

Fig. 6 Minimum ignition energy as a function of dust concentration in different particle diameters

Oxygen concentration is equal to 40% as in experimental conditions [19], the gained results show a reasonable compatibility, but for air (Oxygen concentration = 21 %) as expected, the flame speed is less than the precedent case. The difference between the results is exclusively because the experiment data were for coal particles with 30% volatile, while our model was presented for char particles burning. Due to little difference between our results and those obtained in [19], it can be concluded that our model over predict the effect of char part in burning of the coal particles.

Figure 4 illustrates the changes of flame propagation speed as a function of particle diameter in different values of dust concentration. Flame speed tends to decrease as particle diameter increases. This is mainly due to decreasing of the char specific surface area over which heat transfer and reaction could occur, which, in turn, creates thicker flame front and thus lower propagation speed. Furthermore, with a rise in the value of particle diameter the rate of change is going to slow down. Therefore, in the case of very low particle diameter, the flame speed is higher. Furthermore, as it is shown in Fig.4, as the dust concentration increases, flame propagation speed tends to increase as well; however, the rate of change in higher concentrations decreases.

Figure 5 illustrates the Flame propagation speed in terms of particle size with the consideration of radiation effect. In comparison with the precedent case (neglecting radiation effect), it can be seen that, as expected, the flame propagation speed is higher. It should be noted that in this case, dust and Oxygen concentration is equal to 1.4 (kg/m3) and 40%, respectively.

The minimum ignition energy for a layer in the presumed discrete media as a function of dust concentration for different particle sizes is demonstrated in Fig. 6. As it is shown, with a rise in dust concentration, minimum ignition energy decreases which is because there would be more fuel to let the flame start propagating. Minimum ignition energy function seems to have asymptotic behaviour beyond a certain big dust concentration. To describe this asymptotic behaviour further investigations are necessary. Moreover, with increasing the particles diameter, and thus increasing their resistance, the minimum ignition energy increases.

4 Conclusions

To develop a combustion model that demonstrate the combustion of char particles, a new thermal model considering the discrete nature of the phenomenon was developed by means of numerical and theoretical approaches. A computer code has been generated in order to study the effects of dust concentration and particle size on flame propagation speed.

The results indicate that increase in the value of dust concentration, boosts the flame propagation speed. Also, as the oxidizer concentration increases, the burning time of coal char particles decreases, so the flame speed will rise. It is shown that as the particle size increases, flame speed decreases and after a certain diameter, the rate of flame speed change tends to decelerate. In addition, minimum ignition energy as a function of dust concentration for different particle diameters is illustrated. It is observed that minimum ignition energy tends to have lower values as the particle size decreases.

The results, compared with some experimental data, demonstrated that the new model is an effective model for the estimation of flame front speed in various dust concentrations under different initial conditions.

It should be noted that the present research can be extended to a condition that oxidizers have velocities; therefore, convection terms should be added to the governing equations. The aforesaid suggestion is an important topic for counter flow combustion applications.

Nomenclature

A_p	Surface- area of the particle
C_d	Dust cloud concentration
C_p	Average heat capacity of the particle
$D_{O2,\infty}$	Mass diffusivity of oxygen into the air
d_p	Particle diameter
i, j, k	The number of layers from the specific particle to any particle along each axis
I	Radiation intensity
I_f	Radiation intensity induced from flame boundary to preheat zone
I_b	Black body emission power
K_a	Absorption coefficient
K_s	Scattering coefficient
k_p	Thermal conductivity of particle
L	Space between two adjacent layers
Nu	Nusselt number
n_s	Number of particles per unit volume
n_L	Number of particles in a layer
$P(\Theta,\Phi)$	Phase function for scattering
Q_{rad}	Summation of radiated energy
Q_c	Summation of conducted energy
Q_r	Radiated energy
Q_{Sca}	Efficiency of scattering coefficient
Q_{abs}	Efficiency of absorption coefficient
q_r	Defined in Eq. 19
$\dot{q}$	Rate of heat release of a single particle
R	Ideal gas constant
r	Radial distance
r_p	Particle radius
$r_{i,j,k}$	The space between the target particle and each particle
T_f	Flame temperature
T_p	Particle temperature
T_∞	Ambient temperature
T_s	Temperature of the gas surrounding the particle
T_a	Distribution of temperature around a single burning particle
t	Time
$t_{b_{diff}}$	Burning time of char particle in diffusion controlled regime
$t_{ig,i}$	Ignition time of single particle
x	Distance variable
$Y_{O_{2,\infty}}$	Mass fraction of oxygen in the ambient gas far from the particle surface
α	Thermal diffusivity
ε	Solid particle's emission capability
λ	Heat Conductivity coefficient
Θ	Cone angle, angle from normal of area
τ	Burning time
ρ_p	Apparent density of coal particle
Φ	Circumferential angle
Ω	Solid angle

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