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Numerical simulation of the heterogeneous combustion of dust clouds containing polydisperse porous iron particles

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Abstract In this study, heterogeneous combustion of dust clouds containing polydisperse porous iron particles was numerically investigated. The main aim was to develop a discrete three-dimensional model to quantify the effects of particle size, porosity, cloud concentration, and polydispersity on flame propagation speed. The developed numerical model was validated against experimental data to show its promising accuracy. The modeling results show that increasing the cloud concentration increases flame propagation speed significantly, regardless of the particle size distribution, by about 3 times. Increasing the particle porosity can increase flame propagation remarkably, i.e., for particle sizes in the range of 1–3, 1–10, and 1–30 μm , flame propagation speed was elevated by up to 24.2%, 36.7%, and 22.6%, respectively, when particle porosity increases from 0 to 0.1. However, increasing the particle size itself was found to decrease flame propagation speed as larger particles tend to be more difficult to ignite. For example, when the particle size distribution changes from 1–3 to 1–30 μm , flame propagation speed decreases by a factor of 3.6. These findings serve to improve our understanding of heterogeneous combustion of dust clouds containing polydisperse porous iron particles.

Keywords: Heterogeneous combustion; Iron powder; Polydispersity; Porosity; Numerical simulation; Flame propagation

Nomenclature

Symbols

x, y, z	Cartesian coordinates (m)
Cd	Dust cloud concentration (kg/m^3)
T	Temperature (K)
P	Pressure (atm)

r	Distance from a particle (m)
t	Time (s)
d	Particle diameter (m)
$\dot{q}$	Heat release rate from surface (J/m ² s)
Q	Heat (J)
C	Specific heat (J/kg)
v	Flame propagation speed (m/s)
L	Ignited particle
B	Burning particle
Nu	Nusselt number
$\bar{d}$	Characteristic diameter (m)
k	Thermal conductivity (W/m·K)
f	Non-dimensional particle polydispersity
n	Number of particles
<i>Subscripts</i>	
ave	Average
p	Particle
m	Mixture
a	Air

<i>Fe</i>	Iron
<i>ta</i>	Target particle
∞	Ambient
<i>sur</i>	Surrounding a burning particle
<i>Cond</i>	Conduction
<i>Rad</i>	Radiation
<i>Loss</i>	Heat loss
<i>abs</i>	Absorption
<i>sca</i>	Scattering
ε	Emission capability
<i>igS</i>	Ignition system
<i>Superscripts</i>	
0	Initial
<i>n</i>	Current time step
<i>n + 1</i>	Next time step
<i>Greeks</i>	
α	Thermal diffusivity (m/s ²)
τ	Burning time of particles (s)
φ	Particle porosity

1. Introduction

Combustion is integral to many engineering applications such as aerospace propulsion and industrial power generation [1,2]. The combustion of conventional hydrocarbon fuels, however, can emit pollutants such as NO_x and soot, which are known to be harmful to public health and the environment [3]. Thus, numerous studies have been carried out in search for fuels that are more environmentally friendly [4,5]. Metallic powders are emerging as a promising rival to conventional fossil fuels owing to their cleaner combustion products. Compared with homogeneous combustion, heterogeneous combustion can release more heat per unit volume, which is particularly desirable in high-power mobility applications. As a novel fuel candidate, metallic powders have seen increasing use in heterogeneous combustion applications because their energy density is markedly higher than that of solid hydrocarbon fuels [6]. Among the variety of metallic powders available, micron-sized iron particles are one of the most extensively used in heterogeneous combustion. The merits of using such particles include their widespread availability and proven safety. Despite remarkable progress in recent years, their combustion characteristics are still not completely understood. Nevertheless, a better fundamental understanding of the combustion of micron-sized iron particles is needed if the efficiency of heterogeneous combustion processes is to be further improved.

The heterogeneous combustion of micron-sized iron particles has received considerable attention in recent years. For example, Tang et al. [7] experimentally investigated the combustion of iron dust clouds in argon and helium, and found that the combustion regime of micron-sized iron particles is kinetic but that of millimeter-sized iron particles is diffusive. In another experimental study on the combustion of iron aero-suspensions, Sun et al. [8] reported that combustion occurred on the surface of iron particles without the presence of a gaseous flame. The flame position was determined via luminous spots within the combustion domain. In another experiment, it was found that during the combustion of polydisperse iron dust

clouds, conduction is the dominant heat-transfer mechanism [9]. The lean flammability limits of iron dust clouds for both downward and upward flames have been experimentally measured [10,11]. It was found that as the particle diameter increased, the flame front speed decreased while the quenching distance increased. These experimental studies have profoundly improved our understanding of the heterogeneous combustion of iron dust clouds. However, owing to the recognized challenges of performing measurements under the harsh conditions of heterogeneous combustion, further experiments are needed in order to better understand the complex mechanisms involved.

In the field of combustion, numerical methods are widely used to investigate complex phenomena related to heat release [12] and heat transfer [13]. Such methods can be used to complement experiments for the analysis of the heterogeneous combustion of iron dust clouds. For example, Lee and Stewart [14] developed a numerical model to investigate the combustion of metallic particles with a focus on the non-equilibrium behavior of reactions and phase change. Lam et al. [15] developed a discrete numerical model to explore the combustion of heterogeneous mixtures. Their models, however, did not account for the effects of heat transfer via radiation and polydispersity through particle size distribution. Bidabadi et al. [16] modeled the combustion of iron dust clouds within a one-dimensional discrete framework, and found that the flame front velocity increases with increasing dust-cloud concentration. Hatami et al. [17] used a weighted-residual method to solve the energy equation for the combustion of a single micron-sized iron particle. In this way, they were able to capture the effects of heat transfer via radiation and conduction on the temperature profile of the iron particle. However, they could not analyze the flame front speed or the combustion characteristics of iron powder because their model was limited to only a single particle. Tang et al [7] used a one-dimensional model to numerically simulate the combustion of iron dust clouds with argon–oxygen and helium–oxygen oxidizers. They compared the flame propagation speed calculated by their

1 model with that measured in experiments. For particles smaller than 3 μm , it was found that
2 the flame propagation speed dropped significantly as combustion became kinetically
3 controlled. For larger particles, however, combustion became diffusion controlled. Bozorg et
4 al. [18] developed a numerical model to study the combustion of iron aero-suspensions in a
5 narrow channel, and found that smaller particles have shorter quenching distances.
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12 In real-world situations, iron particles in dust clouds tend to be polydisperse, with a
13 wide distribution of sizes [11]. It is well known that the combustion characteristics of
14 polydisperse particles can be drastically different from those of uniform-sized particles [19].
15 Numerical simulations that assume monodispersity in the particle size could therefore suffer
16 from non-negligible errors. Furthermore, a porous iron particle has a larger surface area than a
17 non-porous iron particle, implying that the former should be easier to ignite than the latter.
18 However, there is relatively little research on the heterogeneous combustion of porous iron
19 powders. To the best of our knowledge, numerical simulations accounting for the effects of
20 both the polydispersity and porosity of metallic particles have yet to be reported, but are needed
21 if further improvements in the efficiency and safety of particle combustion systems are to be
22 achieved.
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40 In this study, we numerically simulated the heterogeneous combustion of polydisperse
41 porous iron particles using a discrete modeling framework [20]. We applied the particle-
42 polydispersity treatment from our previous work [21] in order to model the size non-uniformity
43 of micron-sized iron particles. In the following, we describe the system under study and derive
44 its governing equations. After validating our numerical model with experimental data on the
45 flame propagation speed, we systematically investigated the effects of the particle size
46 distribution and the particle porosity at various dust-cloud concentrations.
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58 **2. System description**

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A polydisperse aero-suspension containing spherical porous iron particles is distributed randomly throughout a rectangular domain. A discrete three-dimensional model, which has been shown to be applicable to the combustion of metallic heterogeneous mixtures including iron aero-suspensions [12], was used to simulate the combustion process. An ignitor plane (marked in red in Fig. 1) provides the energy needed to initiate combustion. When the particles near the ignitor plane reach their ignition temperature, they start to burn. In the preheat zone, the unignited particles near the ignited particles experience a rise in temperature as a result of heat transfer from the latter to the former. Such preheated particles are called target particles. In our modeling framework, the energy equation for all the target particles within the domain is solved at each time step. When a target particle reaches its ignition temperature, it ignites and then preheats its neighboring target particles, causing flame propagation. The flame front at each time step is tracked by monitoring the positions of all the burning particles. Fig. 1 shows an illustration of porous iron particles dispersed throughout the computational domain, alongside the energy balance for a single porous iron particle in the preheat zone. Here Z_{igs} denotes the distance between the ignitor plane and the upper surface of the control volume.

Fig. 1. Illustration of porous iron particles dispersed throughout the computational domain, alongside the energy balance for a single particle in the preheat zone.

3. Governing equations

After the porous iron particles are randomly dispersed throughout the computational domain, the ignitor plane starts to provide the energy needed to initiate flame propagation. Subsequently, the energy equation of each target particle is solved to obtain the temperature at each time step. For a porous target particle (with subscript ta), the energy equation accounting for thermal conduction, radiation and heat losses can be written as

$$\rho_{ta} C_{P,ta} (1 - \varphi) \forall_{ta} \frac{dT_{ta}}{dt} = Q_{Rad,ta} + Q_{Cond,ta} - Q_{Loss,ta} + h_{pf} a_{pf} (T_{ta} - T_f), \quad (1)$$

where ρ_{ta} is the density of the target particle, φ is the particle porosity, $\forall_{ta}$ is the volume of the target particle, $C_{P,ta}$ is the specific heat, h_{pf} is the heat transfer coefficient from the base fluid to the particle, a_{pf} is the specific surface area, and T_f is the temperature of the fluid phase. Moreover, $Q_{Rad,ta}$ is the radiative heat transfer from all the burning particles to the target particle, $Q_{Cond,ta}$ is the conductive heat transfer to the target particle from all the ignited particles and the ignitor plane, and $Q_{Loss,ta}$ is the heat loss from the target particle to the surrounding environment. The temperature of an unignited target particle can be determined by solving Eq. (19) with a finite-difference algorithm, while a_{pf} and h_{pf} can be calculated as [22]:

$$a_{pf} = \frac{6(1-\varphi)}{d_{ta}}, \quad (2)$$

$$h_{pf} = \frac{k_f Nu}{d_{ta}}, \quad (3)$$

where d_{ta} is the diameter of the target particle, k_f is the thermal conductivity, and Nu is the Nusselt number.

For a porous particle with negligible pore-zone thermal conductivity, its effective thermal conductivity can be defined as [23]

$$K_{eff,p} = K_{0,p} \exp\left(\frac{-1.5\varphi}{1-\varphi}\right), \quad (4)$$

where $K_{0,p}$ is the thermal conductivity of the non-porous counterpart. For a two-phase gas-solid mixture, the effective thermal conductivity can be calculated from the Maxwell–Eucken–Bruggeman (MEB) model [24,25] as

$$K_m = \frac{D + \sqrt{D^2 + 2K_{eff,p}K_a}}{2}, \quad (5)$$

where D is defined as

$$D = (2K_{eff,p} - K_a)\varphi(1 - f) + (2K_a - K_{eff,p})(1 - \varphi) \left(\frac{2(1-\varphi)+2\varphi f-1}{2(1-\varphi)}\right), \quad (6)$$

where f represents the structure composition factor, which can be computed with an iterative numerical scheme [24]. Here K_a and $K_{eff,p}$ are the coefficients of thermal conductivity for air and for solid particles, respectively.

The term $Q_{Cond,ta}$ in Eq. (1) captures the conductive heat transfer from all the ignited particles and the ignitor plane to the target particle. The conductive heat transfer from all the ignited particles is found by solving the following energy equation, which is for an ignited particle at distance r and time t

$$\frac{1}{\alpha_m} \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right), \quad (7)$$

where α_m is the thermal diffusivity of the particle-laden mixture, and r is the distance between the target particle and the ignited particle. In the solution of Eq. (7), the following boundary conditions are used [26]

$$K_{eff,p} A_p \frac{\partial}{\partial r} T(r, t) = \dot{q} \times Heaviside(\tau - t) \quad @r = 0.5d_p \quad (8)$$

$$T(\infty, t) = 0, \quad (9)$$

$$T(r, 0) = 0, \quad (10)$$

where $\dot{q}$ is the heat release rate from a burning particle. Given the spherical geometry of the particles, $\dot{q}$ can be expressed as $\dot{q} = K_{eff,p} A_p / r_p (T_f - T_\infty)$ as per Ref. [27], where T_f is the flame temperature, $K_{eff,p}$ is the effective thermal conductivity of the particles, A_p is the particle surface area, and r_p is the particle radius. The temperature of an ignited particle can thus be found by solving Eq. (7) subject to the boundary conditions in Eqs. (8–10), as per Ref. [26]

$$T_{c,ta}(r, t) = (T_f - T_\infty) \frac{d_p}{2r} \left[\operatorname{erfc} \left(\sqrt{\frac{(r - 0.5d_p)^2}{4\alpha_m t}} \right) - Heaviside(t - \tau) \operatorname{erfc} \left(\sqrt{\frac{(r - 0.5d_p)^2}{4\alpha_m (t - \tau)}} \right) \right]. \quad (11)$$

In other words, $T_{c,ta}(r, t)$ of Eq. (11) is the temperature of a target particle at distance r from an ignited particle. Moreover, $r_{ig,ta}$ is the distance from an ignited particle (ig) to a target particle (ta). The superposition principle can be used to calculate the total conductive heat transfer from all the ignited particles to the target particle. Consequently, $Q_{Cond,ta}$ from all the ignited particles up to time t is given as

$$T_{Sur,ta}(t) = \sum_{ig=1}^n T_{c,ta}(r_{ig,ta}, t). \quad (12)$$

As mentioned earlier, an ignitor plane is positioned at the top of the computational domain to provide the necessary initiation energy. The ignitor plane is mounted at a vertical

distance of Z_{igs} above the upper surface of the control volume (see Fig. 1). To determine the portion of thermal conduction from the ignitor plane to $Q_{Cond,ta}$ in Eq. (1), it is necessary to compute the temperature rise of a target particle due to the energy supplied by the ignitor plane. The transient energy equation, which determines the temperature of a given region in the domain at a distance r from the ignitor plane, is given as

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T_{igs,ta}(r,t)}{\partial r} \right) = \frac{1}{\alpha_m} \frac{\partial T_{igs,ta}(r,t)}{\partial t}, \quad (13)$$

where α_m is the thermal diffusivity of the mixture, and r is the distance from the target particle to the ignition source. If the energy from the ignitor plane is assumed to be released over a short time scale, then the corresponding boundary conditions for Eq. (14) are

$$\begin{aligned} k_m \frac{\partial}{\partial r} T_{igs,ta}(r,t) &= \frac{1}{2} q_{igs} \times \delta(t) \quad @ \quad r=0 \\ T_{igs,ta}(r,0) &= 0 \end{aligned} \quad (14)$$

where q_{igs} is the energy released from the ignition system, and $\delta(t)$ is the Dirac delta function.

If it is assumed that the ignitor plane preheats the particles dispersed in the domain during time t_{igs} , the solution of Eq. (14) can be found via

$$T_{igs,ta}(r_{ta,igs}, t_{igs}) = \frac{q_{igs} \alpha_m}{k_m} \frac{1}{\sqrt{(\pi \alpha_m t_{igs})^3}} \exp\left(\frac{-r_{ta,igs}^2}{4 \alpha_m t_{igs}}\right). \quad (15)$$

Considering the effects of both the ignited particles and the ignitor plane, it is convenient to express the spatiotemporal temperature correlation of a target particle as

$$T_{Sur,ta}(t) = T_{igs,ta}(z_{igs}, t_{igs}) + \sum_{ig=1}^n T_{c,ta}(r_{ig,ta}, t), \quad (16)$$

where z is the z -direction distance from the ignitor plane to the target particle, $T_{c,ta}$ is the temperature rise of the target particle due to heat transfer from the ignited particles (see Eq. (11)), and t_{igs} is the time over which the particles are preheated by the ignitor plane. As all the

particles are assumed to be spherical in shape, Nu takes on a constant value of 2. For a target particle, the conductive heat transfer is given as [26]

$$Q_{Cond,ta} = \frac{2k_m A_{ta}}{d_{ta}} (T_{Sur,ta} - T_{ta}). \quad (17)$$

In Eq. (17), T_{ta} is the temperature of the target particle (ta) at time t , and is evaluated after the energy equation is discretized for particle ta .

To find $Q_{Rad,ta}$ in Eq. (1), the radiative heat emitted from all the burning particles near the target particle (ta) must be included. Assuming that the particle-laden mixture is a gray body and that all the particles are spherical in shape, it is possible to express the absorption and scattering coefficients as [18]

$$k_{abs} = \frac{\pi \bar{d}_p^2 n_s}{4} \bar{\epsilon}, \quad (18)$$

$$k_s = \frac{\pi \bar{d}_p^2 n_s}{4} (1 - \bar{\epsilon}), \quad (19)$$

where $\bar{\epsilon}$ is the average particle emissivity, $\bar{d}_p^2$ is the average diameter of the polydisperse particles, and n_s is the number of particles in a unit volume. The radiative heat released from a burning particle b to its neighboring target particle at a distance $r_{b,ta}$ can be written as [18]

$$q_{Rad,b,ta} = \frac{k_{abs}^2}{k_{abs} + k_s} \frac{\sigma \bar{T}_f^4}{n_s \pi} e^{-(k_{abs} + k_s) r_{b,ta}}, \quad (20)$$

where σ is the Stefan–Boltzmann constant, $r_{b,ta}$ is the distance between a burning particle and the target particle, and $\bar{T}_f$ is the average flame temperature of particles dispersed in a unit volume. To derive an explicit expression for $Q_{Rad,ta}$, it is necessary to consider the effect of all the burning particles near the target particle. When n_{nb} particles around the target particle are burning at time t , $Q_{Rad,ta}$ can be calculated as

$$Q_{Rad,ta} = \sum_{b=1}^{n_{nb}} q_{Rad,b,ta}. \quad (21)$$

In Eq. (1), $Q_{Loss,ta}$ is the radiative heat loss from the target particle to the surrounding environment and can be calculated via [28]

$$Q_{Loss,ta} = \pi d_{ta}^2 \sigma \epsilon_{ta} (T_{ta}^4 - T_{\infty}^4). \quad (22)$$

4. Particle distribution

In this study, polydisperse porous iron particles are distributed randomly throughout the domain. The average dust-cloud concentration is given by Cd_{av} . To create a particle-air mixture containing different particle sizes, we use the Nukiyama–Tanasawa distribution with the following density function [29]

$$f_0(d_j) = c_1 d_j^{c_2} \exp(-c_3 d_j^{c_4}), \quad (23)$$

where c_1 , c_2 , c_3 and c_4 are the distribution coefficients, which have the constraint $c_4 \geq c_3$. The ratio of the number of particles with diameter d_j to the total number of particles in the domain is given as

$$\frac{f_0(d_j)}{f_t} = \frac{f_0(d_j)}{\sum_{j=1}^N f_0(d_j)}, \quad (24)$$

where N is the number of discrete diameter values.

5. Numerical procedure

The numerical procedure used in this study consists of two stages. In the first stage, particles are dispersed randomly throughout the computational domain as per Eq. (25) such that a chosen average dust-cloud concentration is achieved. The dust cloud is assumed to have N distinguishing particle diameters. After the polydisperse particles are randomly dispersed, the ignitor plane preheats the mixture over the time interval $t_{ig,s}$. The first set of particles to be ignited are those closest to the ignitor plane, particularly those with smaller diameters and

hence lower ignition temperatures. These particles start to preheat the surrounding unignited particles, i.e. target particles. The temperature of all the target particles is calculated at all time steps. When a target particle reaches its ignition temperature, it starts to burn, preheating other target particles. This is the mechanism by which the flame propagates through the dust cloud. The details of this model can be found in Refs. [19,30].

Under specific conditions, the combustion of micron-sized iron particles is controlled by diffusion [31,32]. Here, a one-stage combustion model is used

For a single iron particle of diameter d_p , the burning time can be calculated as [33]

$$\tau = \frac{\rho_{Fe} d_p^2}{8\rho_{\infty} D_{O_2, \infty} \ln(1 + \nu Y_{O_2, \infty})}, \quad (26)$$

where ρ_{∞} is the density of ambient air, $D_{O_2, \infty}$ is the oxygen mass diffusivity, $Y_{O_2, \infty}$ is the oxygen mass fraction, and ν is the mass stoichiometric index. Table 1 lists the parameters used in this study. From the average temperature of the domain, the thermophysical properties of air are calculated at each time step based on the values in Ref. [34].

Table 1
Thermophysical properties and reaction parameters of iron particles.

Properties	Value	Unit	Ref
ρ_{Fe}	7860	kg/m ³	[34]
$c_{p, Fe}$	447	J/kg · K	[34]
k_{Fe}	80.2	W/m · K	[34]
ϵ_{Fe}	0.505	-	[35]
$T_{ig, Fe}$	900	K	[36]
$T_{f, Fe}$	1990	K	[34]
ν	0.2846	-	[32]
$Y_{O_2, \infty}$	0.233	-	[32]
ρ_{∞}	1.161	kg/m ³	
$D_{O_2, \infty}$	22.5×10 ⁻⁶	m ² /s	[34]

T_{∞}	300	K
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Flame propagation speed is a fundamental quantity of heterogeneous combustion. In the present model, it is defined as the speed at which the flame front moves through the dust cloud, and is calculated based on the positions of the burning particles at each time step as

$$v_z = \frac{(z_{ave}^{n+1} - z_{ave}^n)}{\Delta t}, \quad (27)$$

where z_{ave} is the average position of all the burning particles at each time step. The superscripts $n+1$ and n denote the next time step and the current time step, respectively. The time series of v_z is then averaged over the total simulation time and is reported as the time-averaged flame propagation speed of the dust cloud.

6. Results and discussion

In this section, the flame propagation speed in the heterogeneous combustion of polydisperse porous iron particles is examined, with a focus on the effects of the particle size distribution, the particle porosity, and the average dust-cloud concentration.

6.1. Experimental validation

First, predictions from our numerical model were validated against experimental data from the literature. In our study, polydisperse porous iron particles are randomly distributed in such a way as to reproduce the same particle size distribution as in the experiments of Sun et al. [37]. To determine a suitable distribution function, we identify the parameters in the Nukiyama–Tanasawa distribution (c_1 , c_2 , c_3 and c_4 in Eq. (23)) using particle swarm optimization and a genetic algorithm (PSO-GA) [38]; the numerical values of these coefficients are listed in table 2. Figure 2 compares the particle size (diameter) distribution of our model

against that measured in the experiments of Sun et al. [37]. It can be seen that there is good agreement between the two particle size distributions.

Table 2.

Coefficients of the Nukiyama–Tanasawa distribution computed via PSO-GA.

c_1	c_2	c_3	c_4
1.2592	12.0072	6.4738	0.7700

Fig. 2. Particle size (diameter) distribution used in the present study (blue bars), and its comparison with the distribution measured in the experiment of Ref. [37] (yellow markers).

The particle size distribution shown in Fig. 2 is used to validate our numerical model. The time-averaged flame propagation speed is computed for various dust-cloud concentrations, and is compared with the corresponding experimental values reported by Sun et al. [37]. This comparison is shown in Fig. 3. It can be seen that the model predictions are in good agreement with the experimental data when the dust-cloud concentration is less than around 1.0 kg/m^3 . When the dust-cloud concentration is higher than this threshold, however, the model over-

predicts the flame propagation speed. This is possibly because, at high dust-cloud concentrations, agglomeration of micron-sized particles may have been significant in the experiments, thereby reducing the flame propagation speed; such an agglomeration-induced effect on combustion is not accounted for by our numerical model. Nevertheless, it can still be concluded that the accuracy of our numerical model is acceptable, provided that the dust-cloud concentration remains below 1.0 kg/m^3 .

Fig. 3. Comparison of the time-averaged flame propagation speeds between our numerical model and the experiment of Sun et al. [37] at various dust-cloud concentrations.

6.2. Flame propagation behavior

To demonstrate the effect of particle porosity, we examine the flame propagation behavior in a dust cloud containing porous particles and compare it with that in a dust cloud containing non-porous particles. In both the porous and non-porous cases, the average dust-cloud concentration is fixed at $Cd_{av} = 0.9 \text{ kg/m}^3$. The particles have diameters ranging from 1 to 10 microns, with a porosity of 0.06. The particle size distribution of the dust cloud is the same as that in Fig. 4.

Fig. 4. Particle size distribution of a polydisperse iron dust cloud with particle diameters ranging from 1 to 10 μm .

The instantaneous (i.e. temporal) and time-averaged flame propagation speeds of the porous and non-porous dust clouds are shown in Fig. 5(A) and Fig. 5(B). It can be seen that, for both dust clouds, there are significant fluctuations of the instantaneous flame propagation speed about its time-averaged value; these fluctuations can be up to around $\pm 30\%$ of the time-averaged value. The fluctuations are believed to be due to the random particle distribution and polydispersity of the dust cloud. Recall that the dust cloud contains particles of different sizes, which have different ignition temperatures and hence they ignite at different times. Smaller particles tend to ignite ahead of the average flame front position, whereas larger particles tend to ignite behind the average flame front position. As a result, the overall time trace of the flame speed exhibits fluctuations based on the precise number of small and large particles ignited in the vicinity of the flame front. Finally, the time-averaged flame propagation speed of the porous dust cloud (0.2218 m/s) is around 9% higher than that of the non-porous dust cloud (0.2043 m/s).

(A)

(B)

Fig. 5. Instantaneous (i.e. temporal) and time-averaged flame propagation speeds for iron dust clouds with particle diameters ranging from 1 to 10 μm : (A) a porous dust cloud with a porosity of 0.06, and (B) a non-porous dust cloud.

The cause of the higher flame propagation speed in the porous dust cloud relative to the non-porous dust cloud can be understood by examining Fig. 6(A)-(C) and Fig. 7(A)-(C). These figures show, respectively, a flame propagating through a porous dust cloud and one propagating through a non-porous dust cloud. It can be seen that the effective number of iron particles in the non-porous dust cloud is lower than that in the porous dust cloud. Thus, at each

time step, the number of ignited particles is lower in the non-porous case than in the porous case. This results in fewer thermal sources to preheat the target particles, thereby reducing the speed at which the flame propagates through the non-porous dust cloud. Although increasing the particle porosity can decrease the thermal conductivity, the greater effective number of dispersed particles counteracts this effect, leading to faster flame propagation through the porous dust cloud.

Figure 6(D)-(F) shows the average temperature profiles of iron particles ignited at $t = 0.0112045$ s, 0.16605 s, and 0.22007 s, respectively, in a non-porous dust cloud; only data for the N_n particles shaded in red in Fig. 6(A)-(C) are shown. Similarly, Fig. 7(D)-(F) shows the average temperature profiles in a porous dust cloud with a particle porosity of 0.06. In both cases, the temperature profiles correspond to the flame fronts highlighted in Fig. 6(A)-(C) and Fig. 7(A)-(C). Before time t , the particles are in the preheat zone and are yet to ignite. At time t , the particles reach their ignition temperature and ignite. After time t , the particles tend towards the flame temperature but then cool down as time evolves because they lose heat to the surroundings via radiative and convective heat transfer. Comparing Fig. 6(D)-(F) with Fig. 7(D)-(F), it can be seen that, before the porous particles are ignited at time t , their temperatures are higher than those of the non-porous particles. This is because, at the same average dust-cloud concentration, the effective number of porous particles is higher than that of non-porous particles. Consequently, at each time step, there are more ignited particles available to preheat the unignited neighboring particles in the porous dust cloud than those in the non-porous dust cloud, as evidenced in Fig. 7(A)-(C).

(A)

(D)

(B)

(E)

(C)

(F)

Fig. 6. (A)-(C) Flame propagation through a polydisperse iron dust cloud containing non-porous particles with diameters ranging from 1 to 10 μm and an average concentration of $Cd_{av} = 0.9 \text{ kg/m}^3$. The quantities N_n , N_p , N_0 , N_q , and N_u refer to the number of igniting particles, preheated particles, particles ignited at $t = 0 \text{ s}$ by the ignitor plane, quenched particles, and un-ignited particles, respectively; (D)-(F) temporal evolution of the average temperature of particles ignited at t .

(A)

(D)

(B)

(E)

(C)

(F)

Fig. 7. (A)-(C) Flame propagation through a polydisperse iron dust cloud containing porous particles with diameters ranging from 1 to 10 μm , a porosity of 0.06, and an average concentration of $Cd_{av} = 0.9 \text{ kg/m}^3$. The quantities N_n , N_p , N_0 , N_q , and N_u refer to the

number of igniting particles, preheated particles, particles ignited at $t = 0$ s by the ignitor plane, quenched particles, and un-ignited particles, respectively; (D)-(F) temporal evolution of the average temperature of particles ignited at t .

Figure 8 shows the time-averaged flame propagation speed as a function of the dust-cloud concentration (Cd_{av}) for both non-porous particles and for particles with a porosity of 0.06. When $Cd_{av} < 0.9$ kg/m³, the difference in time-averaged flame propagation speed between the two cases is moderate. For example, the average difference between the two cases is 11.67% and 6.67% for $Cd_{av} = 0.75$ and 0.85, respectively. However, when $Cd_{av} > 0.9$ kg/m³, the difference in time-averaged flame propagation speed increases markedly by up to 29%. This is because increasing Cd_{av} increases the surface area of the porous articles more than it does the non-porous particles. In turn, this increases the number of ignited particles available to act as thermal sources, providing further preheating for faster flame propagation.

Fig. 8. Time-averaged flame propagation speed of polydisperse iron dust clouds containing particles with diameters ranging from 1 to 10 μ m. The data are shown as a function of the

dust-cloud concentration, for both non-porous particles and for particles with a porosity of 0.06.

6.3. Effects of the particle size distribution, particle porosity and Cd_{av}

In this section, effects of particle size distribution, particle porosity ($\varphi = 0, 0.03, 0.06, 0.08, \text{ and } 0.1$) and dust-cloud concentration ($Cd_{av} = 0.45\text{--}1.2 \text{ kg/m}^3$) on the time-averaged flame propagation speed are explored. Figure 9 shows the particle size distribution for three different ranges of particle diameter: (A) 1–3 μm , (B) 1–10 μm , and (C) 1–30 μm . The corresponding parameters used in the Nukiyama–Tanasawa distribution (Eq. (24)) are respectively: (A) $c_1 = 2, c_2 = 7, c_3 = 2, \text{ and } c_4 = 2$; (B) $c_1 = 0.2, c_2 = 5, c_3 = 0.1, \text{ and } c_4 = 2$; and (C) $c_1 = 0.4, c_2 = 6.5, c_3 = 0.5, \text{ and } c_4 = 1.05$.

(A)

(B)

(C)

Fig. 9. Particle size distribution of polydisperse iron dust clouds: (A) 1–3 μm , (B) 1–10 μm , and (C) 1–30 μm .

Fig. 10. Time-averaged flame propagation speed of polydisperse dust clouds containing iron particles with diameters ranging from 1 to 3 μm . Data are shown as a function of the dust-cloud concentration for different values of particle porosity.

Figure 10 shows the time-averaged flame propagation speed as a function of the dust-cloud concentration (Cd_{av}) for particle diameters ranging from 1 to 3 μm . The corresponding particle size distribution is shown in Fig. 9(A). For both porous and non-porous particles, it is found that the flame propagation speed increases with increasing dust-cloud concentration. The minor fluctuations in the flame propagation speed with Cd_{av} can be attributed to random particle dispersion effects. Moreover, it is found that the flame propagation speed also increases with increasing particle porosity, although this effect is relatively weak and consistent across the entire range of dust-cloud concentrations examined. This occurs because the average particle size is small, so ignition and flame propagation occur relatively quickly, weakening the influence of the particle porosity.

Figure 11 shows the time-averaged flame propagation speed as a function of the dust-cloud concentration (Cd_{av}) for particle diameters ranging from 1 to 10 μm . The corresponding particle size distribution is shown in Fig. 9(B). Over the entire range of dust-cloud concentrations examined, the flame propagation speed of the 1–10 μm particles (Fig. 11) is found to be significantly lower than that of the 1–3 μm particles (Fig. 10). As in the previous case with smaller particles (Fig. 10), here the flame propagation speed increases with increasing dust-cloud concentration. As the particle porosity increases, the flame propagation speed also increases, although this effect is more pronounced at high dust-cloud concentrations ($\varphi > 0.9 \text{ kg/m}^3$) than it is at low dust-cloud concentrations ($\varphi < 0.9 \text{ kg/m}^3$). The reason behind this difference was discussed in Fig. 8.

Fig. 11. Time-averaged flame propagation speed of polydisperse dust clouds containing iron particles with diameters ranging from 1 to 10 μm . Data are shown as a function of the dust-cloud concentration for different values of particle porosity.

Figure 12 shows the time-averaged flame propagation speed as a function of the dust-cloud concentration (Cd_{av}) for particle diameters ranging from 1 to 30 μm . The corresponding

particle size distribution is shown in Fig. 9(C). It is found that the flame propagation speed experiences a further reduction in comparison with that observed in the previous cases involving smaller particles: Fig. 10 (1–3 μm particles) and Fig. 11 (1–10 μm particles). Although the overall trends in the flame propagation speed are similar to those observed in Fig. 11, the critical value of the dust-cloud concentration above which particle porosity effects become significant appears to have decreased to 0.8 kg/m^3 . The reason for this is that, as the particles get bigger, they become more difficult to ignite, enhancing the sensitivity of the flame propagation speed to variations in the dust-cloud concentration and in the particle porosity.

Fig. 12. Time-averaged flame propagation speed of polydisperse dust clouds containing iron particles with diameters ranging from 1 to 30 μm . Data are shown as a function of the dust-cloud concentration for different values of particle porosity.

7. Conclusions

In this study, the heterogeneous combustion of dust clouds containing polydisperse porous iron particles was numerically investigated. The particles were randomly dispersed throughout the computational domain. For a target particle in the preheat zone, the conductive

and radiative heat transfer from neighboring burning particles and the heat loss to the domain were taken into account. The flame propagation speed was computed for dust-cloud concentrations ranging from $\varphi = 0.45$ to 1.2 kg/m^3 . The effects of the particle porosity on the flame propagation speed were systematically explored for different particle size distributions and different dust-cloud concentrations. The main findings are as follows:

- For all particle size distributions, increasing dust-cloud concentration was found to increase flame propagation speed. For example, when particle porosity was 0.06, increasing dust-cloud concentration from 0.45 to 1.2 kg/m^3 leads to the increases in flame propagation speed by factors of 3.35, 2.92 and 5.12 in dust clouds containing particle size distribution of 1–3, 1–10 and 1–30 μm , respectively.
- At any given dust-cloud concentration, increasing average particle size was found to decrease flame propagation speed. For example, the flame propagation speed of a dust cloud containing particle size distribution of 1–3 μm is nearly 3.6 times that of a dust cloud containing particle size distribution of 1–30 μm .
- Increasing particle porosity was found to increase flame propagation speed, particularly at high dust-cloud concentrations. For example, increasing particle porosity from 0 to 0.1 leads to the increases in flame propagation speed by up to 24.2%, 36.7%, and 22.6% in dust clouds containing particle size distribution of 1–3, 1–10 and 1–30 μm , respectively.

Future extension of this work can be done in several ways. For example, numerical simulations can be performed to investigate the combustion of dust clouds in a narrow channel to quantify the quenching distance of different particle mixtures. Another open area can be investigation of the influence of injection velocity of the particles or the use of particles with multi-modal size distributions.

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- A 3D model was used to simulate combustion of polydisperse porous iron dust clouds
- Accuracy of the derived numerical model was proved to be promising
- Flame speed of the 1–3 μm group is nearly 3.6 times that of the 1–30 μm group
- Increasing cloud concentration from 0.45 to 1.2 kg/m^3 elevates flame speed by 290%
- Increasing particle porosity from 0 to 0.1 increases flame speed by up to 36.7%

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Simulation results