On conditions for self-sustained combustion of pulverised coal particle-laden mixtures following localised forced ignition: A Direct Numerical Simulation analysis

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1 Introduction

Numerical simulations are playing an increasingly important role in the analysis of coal combustion as a result of the recent advances in high performance computing. Luo et al. [1] recently carried out Direct Numerical Simulations (DNS) of turbulent coal particle-laden mixtures. In the absence of an adequate thermochemical representation of the volatile gas, Luo et al. [1] considered the volatile gas released from the coal to have the properties of methane, treating the coal-particles as point sources, and tracking them in a Lagrangian manner. Recently, Brosh and Chakraborty [2] used three-dimensional DNS for the carrier phase to analyse the effects of particle loading (i.e. particle equivalence ratio, Φ_p , which was defined based on the volatile fuel available in the particulate phase), equivalence ratio of primary volatile fuel in the background gas, Φ , and root-mean-square turbulent velocity fluctuation, u', on the early stages of combustion following localised forced ignition of pulverised coal particle-laden mixtures. This paper extends the analysis of Brosh and Chakraborty [2] to analyse the influences of micro-mixing on the extent of burning during the early stages of combustion following successful ignition. The rate of micro-mixing is determined by the scalar dissipation rate and its effects on the extent of burning in coal particle-laden mixtures are yet to be analysed in the existing literature, despite the fact that the scalar dissipation rate is known to have important influences in droplet-laden combustion processes [3,4]. The present analysis addresses the aforementioned gap by carrying out three-dimensional DNS simulations of localised forced ignition of pulverised coal particle-laden mixtures for a range different values of Φ_n , Φ and u' for different particle diameters, a_n .

2 Mathematical background and numerical implementation

In the absence of an accurate thermochemical model of the form $C_x H_y O_z$ for the volatile matter released by coal, this work follows a previous analysis [1] in which the volatile matter was treated instead as CH_4 .

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A two-step chemical reaction was employed to describe CH_4 -air combustion [2]. Standard Lagrangian transport equations for coal particles account for mass loss due to devolatilisation and char oxidation, momentum change due to drag and energy loss or gain due to convection, devolatilisation, char oxidation and radiation:

$$d\vec{x}_p/dt = \vec{v}_p \tag{1}$$

$$d\vec{v}_{p}/dt = 18C_{d}\mu_{g}(\vec{u} - \vec{v}_{p})/(\rho_{p}a_{p}^{2})$$
(2)

$$dm_p/dt = \dot{m}_v + \dot{m}_{ch} \tag{3}$$

$$\rho_p \left(\pi a_p^3/6\right) C_{pp} \left(dT_p/dt\right) = \left(q_{rad}^{\prime\prime\prime}\right)_p + \pi a_p \mu_g N u_p C_{pg} \left(T_g - T_p\right) / P r_g + \dot{m}_{v1} h_{v1} + \dot{m}_{v2} h_{v2} + \dot{m}_{chA} h_{chA} + \dot{m}_{chB} h_{chB} + \dot{m}_{chC} h_{chC}$$
(4)

where \vec{x}_p , \vec{v}_p , ρ_p , a_p and m_p are particle location, velocity, density, diameter and mass respectively for each particle, p, and μ_g , \vec{u} , and C_d are the fluid viscosity and velocity vector and the particle drag coefficient respectively, where $C_d = 24(1 + Re_p^{0.687})/Re_p$ in which $Re_p = \rho_p a_p |\vec{u} - \vec{v}_p|/\mu_g$ is the particle Reynolds number. \dot{m}_v and \dot{m}_{ch} are the rate of change of mass due to devolatilisation and char oxidation respectively. Here coal particles are preheated and are, thus, free of moisture. C_{pp} is the specific heat capacity of the coal particle p, and the radiation heat flux was evaluated using the Discrete Ordinate Method (DOM), with an S₈ approximation [5] in the following manner: $(q_{rad}^{\prime\prime\prime})_p =$ $\epsilon_p (\Theta_r^4 - T_p^4)$ with Θ_r being the radiation temperature evaluated from the radiation intensity $\Theta_r =$ $(I/4\sigma)^{1/4}$ where I is the intensity and $\sigma = 5.67 \times 10^{-8} W/m^2 K^4$ is the Stefan-Boltzmann constant. The particle emissivity ϵ_p varied from 1 (fresh particle) to 0.6 (fully burnt particle) following [6] as $\epsilon_p = 0.6 + 0.4 (m_v + m_{ch})/(m_{v,0} + m_{ch,0})$, where $m_{v,0}$ and $m_{ch,0}$ are the initial volatile gas and char content of the particle. Convective heat transfer from the particle is accounted for by the Ranz-Marshall expression for Nusselt number $Nu_p = 2 + 0.6Re_p^{0.5}Pr_g^{0.33}$ where Pr_g is the Prandtl number of the gaseous phase.

A two-way coupling between the phases was implemented by interpolating fluid properties from the Eulerian carrier phase to the Lagrangian particulate phase and extrapolating particle properties in the opposite direction. The Eulerian transport equations for the general primitive variable φ are [1-4]:

$$\partial(\rho_g \varphi) / \partial t + \partial(\rho_g u_j \varphi) / \partial x_j = \nabla \cdot \left[\left(\mu_g / \sigma_\varphi \right) \nabla \varphi \right] + \dot{S}_{\varphi g} + \dot{S}_{\varphi p} + \dot{S}_{\varphi ch} + \dot{S}_{\varphi sp} + \dot{S}_{\varphi rad}$$
(5)

where ρ_q is the gas density, and σ_{φ} is the Schmidt number associated with φ . The variable $\varphi =$ $\{1, u_i, e, Y_\alpha\}$ for mass, momentum, energy and species conservation respectively, where e = $\int_{T_{ref}}^{T} C_{\nu g} dT + (u_k u_k/2)$ is the specific stagnation internal energy, in which \hat{T} and T_{ref} are the instantaneous gas and reference temperatures respectively. Equation 5 contains source terms due to the gaseous reaction $(\dot{S}_{\varphi g})$, particles $(\dot{S}_{\varphi p})$, char $(\dot{S}_{\varphi ch})$, spark ignition $(\dot{S}_{\varphi sp})$ and radiation $(\dot{S}_{\varphi rad})$. The source term due to particles is evaluated as [1-4] $\dot{S}_{\varphi p} = -(\Delta V)^{-1} \sum_{p} d(m_p \varphi_p)/dt$, where ΔV is the cell volume. The energy deposition during the ignition stage of the simulation is modelled as [2-4] $\dot{S}_{\varphi sp} = q^{\prime\prime\prime}(r) = A_q \exp(-r^2/2R^2)$, where r is the radial distance from the centre of the ignitor (located at the centre of the domain) and R is taken to be $1.73l_f$, in which $l_f = \alpha_{T0}/S_{b(\Phi=1)}$ is the Zel'dovich flame thickness for the stoichiometric volatile fuel-air mixture, where $S_{b(\Phi=1)}$ is the unstrained laminar burning velocity of the stoichiometric mixture of volatile fuel and air. The constant A_q is determined by $\dot{Q} = \int_V q^{\prime\prime\prime} dV$, where the ignition power, \dot{Q} is defined as $\dot{Q} =$ $a_{sp}\rho_0 C_P \tau T_0(\{4/3\}\pi l_f^3)[\{H(t) - H(t - t_{sp})\}/t_{sp}],$ where $\tau = (T_{ad(\Phi=1)} - T_0)/T_0$ is the heat release parameter with T_0 and $T_{ad(\phi=1)}$ being the initial reactant temperature and the adiabatic flame temperature of the stoichiometric volatile fuel-air mixture respectively, a_{sp} is a parameter which determines the total energy deposited by the ignitor. Based on a previous study [2], $a_{sp} = 25.72$ and

25th ICDERS - August 2-7, 2015 - Leeds

Brosh, T.

 $\tau = 3.0$ are taken for the current analysis and the Lewis number of all species is taken to be unity. The energy deposition duration t_{sp} is expressed as: $t_{sp} = b_{sp}t_f$ where $t_f = l_f/S_{b(\phi=1)}$ and the parameter b_{sp} is taken to be 0.2 following previous analyses [2-4]. Radiative heat transfer effects are modelled using the DOM S₈ approximation [5] $\dot{S}_{\varphi rad} = -\kappa_g (4\sigma T_g^4 - \Theta_r^4)$, where the absorption and emissivity of the gas are evaluated from grey gas approximation [5] $\kappa_g = 0.2\chi_{CH_4} + 0.1(\chi_{CO_2} + \chi_{H_2O})$, where χ_i is the mole fraction of the *i*th gas. Both $\dot{S}_{\varphi sp}$ and $\dot{S}_{\varphi rad}$ are active only in the energy transport equation. Interested readers are referred to Refs. [1,2] for the modelling of devolatilisation and char oxidation considered in the current analysis.

Parameter	value	Naming convention
a _p	no particles	aO
	$0.12l_{f}$	a1
	$0.18l_{f}$	a2
Φ	0	G0
	0.5	G1
	1	G2
$\Phi_{\rm p}$	0	PO
	0.5	P1
	1	P2
$u'/S_{b(\Phi=1)}$	0	U0
	4	U1
	5	U2
	6	U3

Table 1 . Parametric variation and naming convention

The simulations have been carried out using a three-dimensional compressible DNS code SENGA [2]. The domain is taken to be $33l_f \times 33l_f \times 33l_f$, which is discretized using a uniform Cartesian grid of $200 \times 200 \times 200$ ensuring 10 grid points within the flame of the stoichiometric fuel-air mixture. This grid spacing also resolves the Kolmogorov length scale. All turbulent cases were initialized using a standard pseudo-spectral method for different initial values of u' for a single value of normalised longitudinal integral length scale (i.e. $L_{11}/l_f = 5.2$). Mono-dispersed, preheated (550K) particles were distributed along the domain in x_2 and x_3 directions and over the 70% of the domain length in the x_1 direction around the centre of the domain where the ignitor was placed.

3 Results and discussion

The parametric variation in terms of particle diameter a_p , particle equivalence ratio Φ_p (based on the available volatile fuel in the particulate phase), equivalence ratio (based on gaseous fuel Φ in the background gas) and rms turbulent velocity fluctuation normalised by the unstrained laminar burning velocity $u'/S_{b(\Phi=1)}$ are summarised in Table 1. The temporal variation of the maximal non-dimensional temperature $T_{max} = (\hat{T}_{max} - T_0)/(T_{ad(\Phi=1)} - T_0)$ (where \hat{T} is the instantaneous dimensional temperature) is presented in Fig. 1, which shows a rapid increase in T_{max} with time until $t = t_{sp}$ followed by a slower decrease in T_{max} once the ignitor is switched off. In cases where self-sustained combustion is obtained $\hat{T}_{max} \approx T_{ad(\Phi=1)}$ for $t \gg t_{sp}$, otherwise T_{max} decreases monotonically once the ignitor is switched off (i.e. $t > t_{sp}$) as the heat release due to combustion in these cases is not sufficient to overcome the heat transfer from the hot gas kernel (e.g. cases G1P0a0U1 and G1P1a1U3).

25th ICDERS – August 2-7, 2015 - Leeds



Figure 1. The temporal variation of T_{max} for parametric variations of (a) u', (b) Φ_p and a_p and (c) Φ .



Figure 2. Distribution of primary fuel mass fraction at $t = 1.0t_{sp}$ (1st column) and $t = 10t_{sp}$ (2nd column) and non-dimensional temperature *T* at $t = 1.0t_{sp}$ (3rd column) and $t = 10t_{sp}$ (4th column) in the central x_1 - x_2 plane for G1P1a1U1. The magenta dashed line represent the stoichiometric mixture isosurface (i.e. $\Phi = 1.0$)

The distributions of the mass fraction of primary volatile fuel and non-dimensional temperature in the central mid-plane at different times for case G1P1a1U1 are shown in Fig. 2. Devolatilisation from the preheated particles leads to the release of fuel vapour, but the vapour is rapidly consumed at the centre of the domain due to high local temperature for $t \le t_{sp}$. Figures 1 and 2 show that T_{max} for $t \gg t_{sp}$ is much smaller than at $t = t_{sp}$ and, thus, the consumption rate of primary fuel is smaller for $t \gg t_{sp}$ than at $t = t_{sp}$. As a result the devolatilised fuel is not readily consumed, giving rise to fuel-rich clouds in the vicinity of the hot gas kernel for $t \gg t_{sp}$ (e.g. $t = 10t_{sp}$ in Fig. 2). This behaviour has implications on self-sustained combustion of coal particle-laden mixtures following localised ignition.

The temporal evolution of $\tilde{T} = \langle \rho T \rangle / \langle \rho \rangle$ (<. > indicates spatial averaging) evaluated over the domain is presented in Fig 3 for some selected cases. All cases show the same trend with rapid rise of \check{T} during the energy deposition period. It can be seen from Fig. 3a that an increase in u' gives rise to better mixing of the hot air and devolatilised fuel leading to a more rapid chemical reaction rate and, hence, to an increase in \check{T} with time. However, for high values of u', heat transfer from the hot gas kernel eventually overcomes the chemical heat release rate which leads to flame quenching. Figure 3b shows that for cases with no particles (e.g. G1P0a0U1) there is a more rapid rise in \check{T} (because the particles have higher specific heat than the gas). However, in case G1P0a0U1 the amount of volatile fuel is insufficient to sustain the chemical reaction once the temperature drops (following the switching off of the ignitor) and under this condition T approaches a constant value. It can further be seen from Fig 3b that T assumes smaller values for higher values of Φ_p (compare G1P1a1U1 and G1P2a1U1). This is because the probability of finding highly fuel-rich pockets, where combustion cannot be sustained, increases with increasing Φ_p due to the availability of a high concentration of volatile gas. Also, \check{T} assumes higher values for larger particles because the devolatilisation rate is faster for smaller particles increasing the probability of finding highly fuel-rich incombustible mixtures and leading to an overall reduction in heat release rate. Figure 3c shows that a reduction of Φ leads to higher values of \tilde{T} . The presence of high concentration of volatile fuel in the background gas increases the likelihood of the development of incombustible fuel-rich gas pockets which reduce the magnitude of \check{T} .

The extent of burning can be quantified in the form of total mass of CO, CO_2 and H_2O (i.e. $m_{CO} + m_{CO_2} + m_{H_2O}$) produced due to combustion of volatile fuel. The temporal evolution of $M^* = (m_{CO} + m_{CO_2} + m_{H_2O})/([4/3]\rho_0\pi l_f^3)$ is shown in Fig. 4. It is evident from Fig. 4a that high values of u' result in small values of $(m_{CO} + m_{CO_2} + m_{H_2O})$ for $t \gg t_{sp}$, indicating that the extent of

25th ICDERS - August 2-7, 2015 - Leeds

burning decreases with increasing u'. In the absence of particles more energy is transferred to the fuelair mixture which leads to a more rapid generation of products, but the flame eventually quenches if the mixture is too fuel-lean to sustain combustion. Figure 4a-b show that an increase (decrease) in Φ_p and $\Phi(a_p)$ act to increase the probability of finding incombustible fuel-rich pockets and thus reduces the overall heat release and M^* .



Figure 3. The temporal variation of $\check{T} = \langle \rho T \rangle / \langle \rho \rangle$ for varying (a) u', (b) Φ_p and a_p , and (c) Φ .



Figure 4. The temporal variation of M^* for varying (a) u', (b) Φ_p and a_p , and (c) Φ .

Wandel [4] attempted to predict the probability of flame extinction based on the global mean mixture fraction dissipation rate. Here the mixture fraction, ξ , is defined in terms of the elemental mass fraction of carbon Y_{CF} arising from both primary and secondary fuels in the following manner $\xi =$ $(Y_{CF} - Y_0/s + Y_{0\infty}/s)/(Y_{CF\infty} + Y_{0\infty}/s)$, in which $Y_{CF\infty} = 0.75$ and $Y_{0\infty}/s = 0.233$ are the carbon mass fraction in the pure methane and the oxygen mass fraction in the pure air streams respectively and s = 5.33 is the ratio of the mass of oxygen to the mass of carbon in methane. These values yield the stoichiometric mixture fraction $\xi_{st} = 0.055$. The scalar dissipation rate $N_{\xi\xi}$ of the mixture fraction is defined as $N_{\xi\xi} = D\nabla\xi \cdot \nabla\xi$ with D being the diffusivity of mixture fraction. The temporal evolution of the normalised mixture fraction scalar dissipation rate $\langle N_{\xi\xi} \rangle / N_{ext}$ is shown in Fig. 5, where $N_{ext} =$ $\xi_{st}^2 (1 - \xi_{st})^2 / t_f$. It can be seen from Fig. 5 that, for most cases, $\langle N_{\xi\xi} \rangle / N_{ext}$, increases with time, apart from a small decrease immediately after the ignitor is switched off. Figure 5a shows that $\langle N_{\xi\xi} \rangle$ $/N_{ext}$ increases with increasing u'. Moreover, the small value of $< N_{\xi\xi} > /N_{ext}$ in the case G1P0a0U1 without particles implies that $N_{\xi\xi}/N_{ext}$ in this configuration changes mostly in response to the devolatilisation rate and u'. Figure 5c shows that higher values of $\langle N_{\xi\xi} \rangle / N_{ext}$ are obtained for higher Φ values during the early stages of combustion following ignition. This originates due to high mixture fraction gradient generated due to high rates of devolatilisition at high values of temperature. Once the temperature settles to $\hat{T}_{max} \approx T_{ad(\Phi=1)}$, the values of $\langle N_{\xi\xi} \rangle / N_{ext}$ are dominated by the devolatilisation rate, which is not significantly affected by Φ for values considered here. A comparison between Figs. 1,3-5 suggests that high values of $N_{\xi\xi}/N_{ext}$ have a negative effect on self-sustained combustion following successful ignition. The extent of completion of chemical reaction can be quantified in terms of the reaction progress variable $c = [(1 - \xi)Y_{0\infty} - Y_0]/[(1 - \xi)Y_0]/[(1 - \xi)Y_0]/$ $\max\{0, (\xi_{st} - \xi)/\xi_{st}\}Y_{0\infty}$, which increases monotonically from 0 in unburned gas to 1.0 in fully burned products. The scatter of $N_{\xi\xi}/N_{ext}$ with c for different values of $u'/S_{b(\Phi=1)}$ at $t = 10t_{sp}$ is shown in Fig. 6. It can be seen from Fig. 6 that the low u' cases ,where self-sustained combustion is obtained, exhibit high probability of finding high (low) values of $c (N_{\xi\xi}/N_{ext})$. In contrast, the high u' cases, where flame eventually quenches, show high probability of finding high (small) values of $N_{\xi\xi}/N_{ext}$ (c). 25th ICDERS – August 2-7, 2015 - Leeds 5

Brosh, T.

Figures 5 and 6 suggest that devolatilisation gives rise to high values of $N_{\xi\xi}/N_{ext}$ at the fuel-rich devolatilisation sites where the probability of obtaining high values of *c* is small and thus the cases where the high values of $N_{\xi\xi}$ are obtained are unlikely to exhibit self-sustained combustion when external energy is not added following successful ignition.



Figure 5. The temporal variation of $N_{\xi\xi}/N_{ext}$ for varying (a) u', (b) Φ_p and a_p and (c) Φ .



Figure 6. Scatter of $N_{\xi\xi}/N_{ext}$ with c, colored by joint probability density function for (a) $u'/S_{b(\Phi=1)} = 0$, (b) $u'/S_{b(\Phi=1)} = 4$ and (c) $u'/S_{b(\Phi=1)} = 6$ for cases G1P1a1 ($\Phi = 0.5, \Phi_p = 0.5$ and $a_p = 0.12l_f$).

4 Conclusion

The effects of Φ_p , Φ , a_p and u' on early stages of combustion subsequent to successful ignition have been analysed based on DNS. It has been found that an increase in u' helps to mix the devolatilised fuel with surrounding air, but flame quenches for high values of u'. The mean scalar dissipation rate $N_{\xi\xi}$ of mixture fraction has been found to be strongly affected by u', whereas Φ_p , Φ and a_p have been found to affect the mean value of $N_{\xi\xi}$ through their influences on devolatilisation rate. It has been demonstrated that high values of $N_{\xi\xi}$ are associated with small values of c and the cases which are likely to show high values of $N_{\xi\xi}$ are more prone to flame extinction without the aid of external energy addition following successful ignition.

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