Promotion and Mitigation of Premixed Flame Acceleration in Dusty-Gaseous Environment with Various Combustible Dust Distributions: A Computational Study

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1 Introduction

Accidental explosions of flammable gases due to combustible dust impurities may result in injuries and deaths as well as the destruction of expensive equipment, thereby constituting a serious demand in the industries dealing with explosive materials such as the coalmining industry, which historically has one of the highest fatality and injury rates. While combustion of gaseous fuels has been studied reasonably well as of now, as well as that of combustible dust particles, the process of flame propagation in a combined gaseous-dusty environment, especially with a non-uniform dust distribution in a gas, nowadays still remains almost as an enigma that commands both the fundamental interests and practical relevance.

A planar premixed flame front would propagate, with respect to a fuel mixture, with an unstretched laminar speed S_L, which is a thermal-chemical parameter, but such a planar flame rarely occurs in the practical reality. Indeed, the majority of industrial and laboratory flames are usually corrugated due to turbulence, acoustics, shocks, combustion instabilities, wall friction, in-built obstacles etc. A curved flame front has a larger surface area relative to a planar one; therefore, it consumes more fuel mixture per unit time and releases more heat, thereby propagating faster than the planar flame front, say, with a certain "wrinkled" flame velocity $U_w > S_L$. Consequently, a flame should accelerate with a continuous increase in the flame surface area. In particular, one of the well-known mechanisms of flame acceleration is that by Shelkin [1], associated flame acceleration due to nonslip boundary conditions at the walls. Specifically, as a flame front propagates from a closed tube/channel end, the burning matter expands; it pushes a flow of the fresh fuel mixture; friction at the pipe walls makes the flow non-uniform, which bends the flame front, increasing its velocity and thereby yielding and promoting associated acceleration. The Shelkin idea was subsequently developed and quantified by the analytical formulation and extensive computational simulations of Bychkov *et al.* [2]. However, similar to numerous concomitant studies, the theory and modelling [2] employed the so-called "geometrical" consideration, when the ratio U_w / S_L is analyzed, whereas the entire "thermal-chemistry" of combustion assumed to be immersed in the constant S_L.

This is a conventional theoretical approach, but in the practical reality, the thermal-chemical flame-fuel properties such as S_L may oftentimes experience spatial and temporal variations caused, in particular, by the non-uniform distributions of an equivalence ratio or dust impurity within a coalmine. With the present work, we initiate a systematic study on how such local variations of S_L and of other parameters may influence the global flame evolution. In this particular study, we consider dusty-gaseous environment and test the approach on the example of flame acceleration due to wall friction. Specifically, the computational simulations of the compressible hydrodynamic and combustion equations are performed, with the combustible coal dust particles incorporated into the original CFD platform by means of the classical

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Seshadri formulation [3]. Namely, a real gaseous-dusty environment is replaced by an "effective" gaseous fluid with locally-modified, dust-induced flow and flame parameters. Keeping in mind a coalmine passage as a potential application, we consider flame propagation in a pipe with a large aspect ratio. For simplicity, the two-dimensional (2D) planar Cartesian geometry is employed. Various coal dust concentration distributions are studied: namely, the (a) homogenous, (b) linear, (c) cubic and (d) parabolic ones. While the homogenous distribution simply provides a scaling factor as compared to the gaseous case [2], the non-uniform distributions were anticipated to provide qualitatively new features. In this respect, we have identified the similarity and differences in the evolution of the flame shape morphology and the flame propagation velocity in each case. It is shown that a non-uniform dust distribution may result in an extra distortion or local stabilization of the flame front, which promotes or reduces the total flame front surface area, thereby facilitating or moderating the flame velocity and thus acceleration induced by wall friction.

2 Computational Platform

The core of the computational platform consisted of a fully-compressible, finite-volume Navier-Stokes code solving for the hydrodynamics and combustion equations in gaseous environment. It was adapted to parallel computations and validated on numerous reactive flow and aero-acoustic problems [4-5]. More details about the computational platform can be found in the Ref. [2]. The basic equations read:

$$\frac{\partial}{\partial t}\rho+\frac{\partial}{\partial x_i}\left(\rho u_i\right)=0, \qquad \frac{\partial}{\partial t}\left(\rho u_i\right)+\frac{\partial}{\partial x_j}\left(\rho u_i u_j+\delta_{i,j}P\right)-\gamma_{i,j}=0, \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon+\frac{1}{2}\rho u_i u_j\right)+\frac{\partial}{\partial x_i}\left(\rho u_i h+\frac{1}{2}\rho u_i u_j u_j+q_i-u_j\gamma_{i,j}\right)=0, \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho Y\right)+\frac{\partial}{\partial x_i}\left(\rho u_i Y-\frac{\zeta}{\mathrm{Sc}}\frac{\partial Y}{\partial x_i}\right)=-\frac{\rho Y}{\tau_R}\exp\left(-E_a/R_p T\right), \tag{3}$$

where Y is the mass fraction of the fuel mixture, $\varepsilon=QY+C_v T$ the internal energy, $h=QY+C_p T$ the enthalpy, Q the energy release in the reaction, and C_V, C_P the specific heats at constant volume and pressure, respectively. We consider a single irreversible first-order Arrhenius reaction, with the activation energy E_a and the constant of time dimension τ_R. The stress tensor $\gamma_{i,j}$ and the energy diffusion vector q_i are given by

$$\gamma_{i,j}=\zeta\left(\frac{\partial u_i}{\partial x}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{i,j}\right), \qquad q_i=-\zeta\left(\frac{C_p}{\mathrm{Pr}}\frac{\partial T}{\partial x_i}+\frac{Q}{\mathrm{Sc}}\frac{\partial Y}{\partial x_i}\right), \tag{4}$$

where $\zeta\equiv\rho\nu$ is the dynamic viscosity, Pr and Sc the Prandtl and Schmidt numbers, respectively. The walls are adiabatic, $\hat{n}\cdot\nabla T=0$, and nonslip, $u=0$, where $\hat{n}$ is a normal vector perpendicular to the side walls. Additionally, to avoid weak shock and sound waves, the nonreflecting boundary conditions are selected at the open end of the channel. The classical Zeldovich-Frank-Kamenetsky (ZFK) solution [6] is used for a planar flame front as our initial condition. Later, we implemented the combustible dust particles into this solver by using the Seshadri formulation [3] that expresses the laminar burning velocity, $S_{d,L}$, as a function of local thermal-chemical properties of the gas and coal dust in the form

$$S_{d,L}=\frac{1}{Ze}\sqrt{\frac{2Bk_u}{\rho_u C_T}\exp\left(-\frac{E_a}{R_u T_f}\right)}, \qquad Ze=\frac{E_a\left(T_f-T_u\right)}{R_u T_f^2}, \tag{5}$$

where Ze is the Zel'dovich number, and C_T the entire specific heat of the mixture,

$$C_T = C_P + C_s n_s \frac{4\pi r_s^3}{3} \frac{\rho_s}{\rho}, \qquad (6)$$

with C_s being that of the coal dust particles. Here ρ is the density of the mixture, which can be expressed as $\rho = \rho_u + c_s$, where ρ_u is the density of the fresh gas and c_s the concentration of particles. The quantity $n_s = (c_s / \rho_s) / V_s$ is the number of particles per unit volume, with $V_s = 4\pi r_s^3 / 3$ being the volume of a single particle and r_s the radius of this particle. The flame speed is promoted by the effect of volatiles released from the coal particles through the gaseous mixture, which is accounted as an additional fuel source for the combustion process in the reaction zone. As a result, the growth of the equivalence ratio promotes the flame temperature T_f^* and, thereby, the burning velocity $S_{d,L}^*$; see Refs. [3,7] for details.

In this study, we utilize and test the developed computational platform through the analysis of the impact of various combustible dust distributions on the scenario of flame acceleration induced by wall friction. In fact, the coal dust distribution is typically non-uniform in coalmines [8]. Indeed, a stationary dense coal dust layer may spread through the bottom of the channel. Initially, a gaseous-based detonation wave may produce a strong shock that can lift and entrain the dust layer. Later, the shock weakens but the shock-heated air is ignited by the lifted dust [8]. Hence, a secondary combustion process is initiated in the mixture of gaseous methane-air and non-uniform dust. In this manner, a lifted dust layer may resemble a linear, cubic, or even parabolic distribution due to the different energy levels of the complex magnetic forces. In fact, this may justify our choice of dust distributions, specified below, though it is difficult to identify a realistic distribution of coal particles in a coalmine.

The four distributions considered are presented in Fig. 1. First, we employed the uniform coal dust concentration distribution, Fig. 1a, which provided a base model for the computational platform. Subsequently, we considered three non-uniform distributions along the channel as functions of the radial coordinate. In the case of linear coal dust concentration distribution, Fig. 1b, we have the maximum dust concentration, $c_{s,\max}$, at the bottom of the channel and no dust at the top of the channel. By applying the boundary conditions on the linear gradient of non-uniform dust distribution, we end up with the function

$$c_s = c_{s,\max} \left(1 - x / 2R\right). \qquad (7)$$

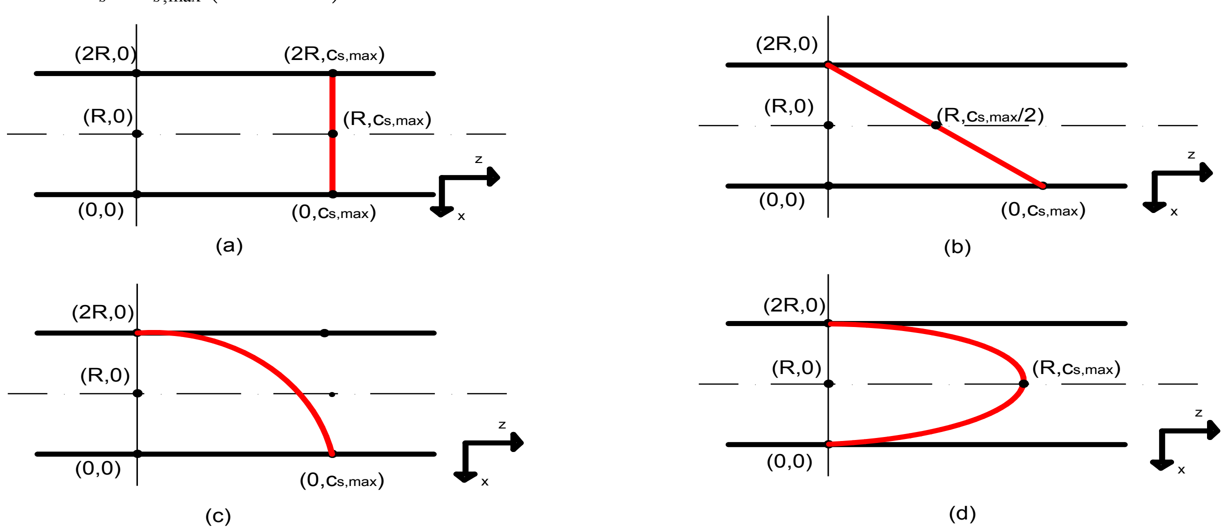

Figure 1. Schematic of the different coal dust concentration distributions:
(a) homogenous; (b) linear; (c) cubic and (d) parabolic.

We also considered a cubic coal dust concentration distribution, Fig. 2c,

$$c_s = c_{s,\max}\left[1-(x/2R)^3\right], \tag{8}$$

and a parabolic one, Fig. 1d,

$$c_s = c_{s,\max}\left[1-4((x-R)/2R)^2\right], \tag{9}$$

where the maximal dust concentration is attained along the centerline, and it is zero (no dust) along the bottom and top of the channel. With $x = 0$, all Eqs. (7) – (9) obviously yield $c_s = c_{s,\max}$ as in Fig. 1a.

In the present simulations, we considered lean ($\phi = 0.7$) methane/air/coal dust combustion, which is relevant to the practical reality. Additionally, a small particle radius, r_S = 10μm, providing an effective equivalence ratio promotion due to fast pyrolysis ability, is used, with a concentration of 120g/m^3. The laminar flame speed for the given equivalence ratio, $\phi = 0.7$, in the absence of dust particles was taken as $S_L = 0.169$ m/s [9]. This value provides realistically slow flame propagation as compared to the speed of sound (the flame Mach number is $Ma = S_L / c_0 = 4.87\times10^{-4}$). In fact, this fame velocity can be calculated by using Eq. (5) with $c_s = 0$ or r_S = 0. The thermal expansion in the burning process is determined by the energy release in the reaction, and it is defined as the fuel-to-burnt matter density ratio, $\Theta = \rho_u / \rho_b$; we took Θ = 6.11, which is related to methane/coal particle burning for the given equivalence ratio, $\phi = 0.7$ [9]. We took the standard ("room") initial pressure and temperature, $P_f = 10^5$ Pa and $T = 300K$. The dynamic viscosity and the Prantdl number were taken as ζ = 1.7×10^{-5} Ns/m^2 and Pr = 1.0, respectively, with the Lewis number being $Le = \mathrm{Pr}/Sc = 1.0753$. The gas phase is considered to be an ideal gas, $P = \rho R_p T / m$, with a constant molecular weight $m = 2.9\times10^{-2}$ kg/mol. The activation energy was chosen as $E_a = 56 R_p T_f$. The flame dynamics is conventionally characterized by the flame Reynolds number

$$\mathrm{Re} = \frac{R S_L^{mean}}{\nu} = \frac{R}{\mathrm{Pr}\, L_f}, \tag{10}$$

where $L_f = 8.65\times10^{-5}\, m$ is the thermal flame thickness and R the channel half-width. It was shown that the effect of non-uniform dust distribution becomes substantial when the channel width is no less than 24 L_f, so we used this value of Re, Re = 24 in the present simulations. The computational mesh size was as large as 0.25 L_f in the axial direction and ~0.5 L_f in the radial direction, which can be considered as a sufficiently refined grid according to our resolution tests performed in the previous works.

3 Results and Discussion

Figure 2 demonstrates the characteristic behavior of an accelerating flame for different dust distributions. Specifically, Fig. 2a shows the scaled flame velocity taken at the channel axis, U_c, scaled by the laminar quantity S_L, versus the scaled time $\tau = tS_L / R$. First of all, we observe that the parabolic dust distribution moderates flame acceleration as compared to the homogeneous case. Also, the plots for the linear and cubic distributions closely resemble each other. We also studied the case of no dust, which showed a similarity to the homogeneous distribution but moderation is higher than that in the parabolic case. In Fig. 2b, the scaled flame front surface area, A_w/2R, is presented versus scaled time $\tau = tS_L / R$. As the flames surface area grows, so does its velocity. In the case of parabolic distribution, the lower flame front surface area moderates flame acceleration as depicted in Fig. 2a.

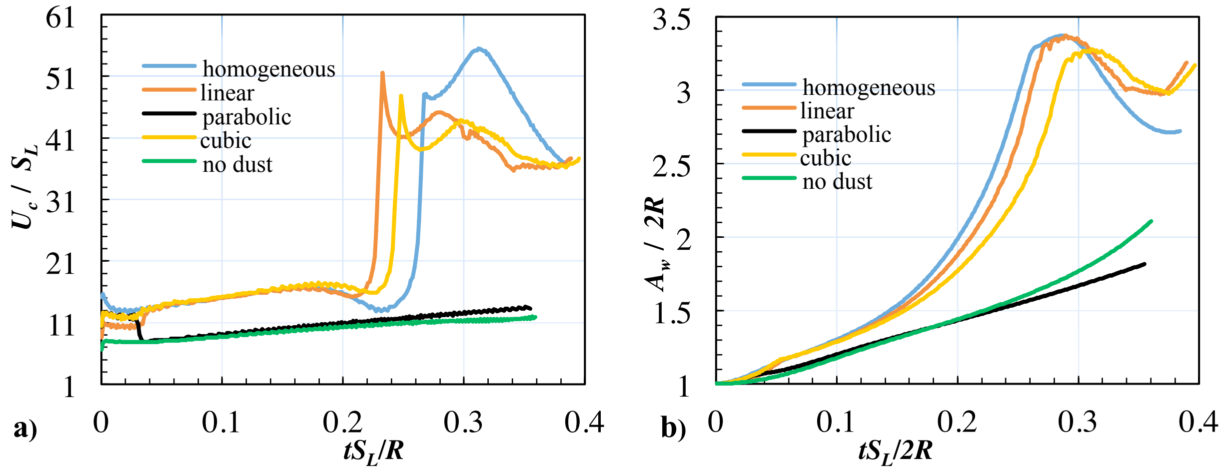

Figure 2. The scaled propagation speed of the flame tip U_c / S_L (a) and the scaled flame surface area $A_w /2R$ (b) versus the scaled time $t\,S_L$ / R for various coal dust concentration distributions.

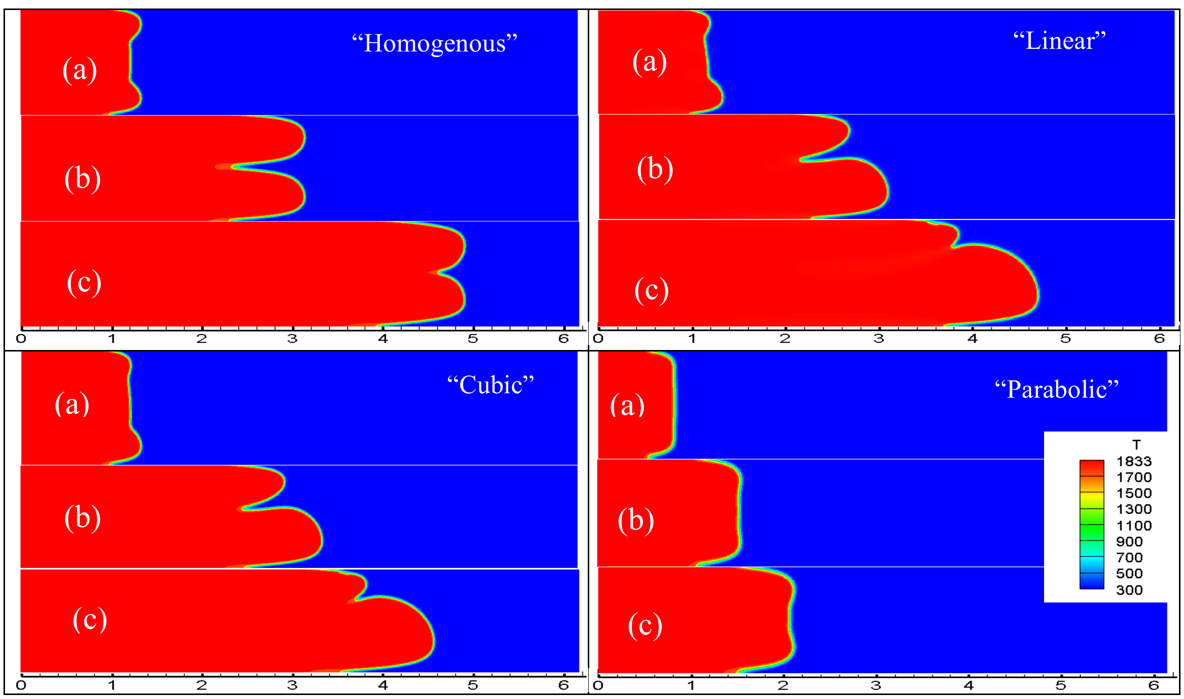

Figure 3. Temperature field evolution in a channel of half-width $R = 24L_f : \tau = 0.15$ (a), $\tau = 0.27$ (b), $\tau = 0.36$ (c).

But what mechanism is responsible for such a trend? In order to answer this question, we investigated the evolution of the flame shape for all distributions at identical time intervals as shown in Fig. 3. For all simulation runs, the flame was initiated in the form of an initially planar front propagating in a semi-open channel from the closed end to the open one. Subsequently, the flame front gets corrugated due to wall friction and thereby non-uniform flow velocity field produced. In the case of a homogeneous distribution, we observe the formation of a trough, which gets stronger with time, but afterwards the center part of the flame accelerates faster than its upper and lower segments; see also Fig. 2a. At the end, only a small through is visible. The origin of the trough may be attributed to the on onset of the hydrodynamic

(Darrieus-Landau; DL) flame instability inherent for the considered Reynolds number [2]. The non-uniform distribution of the coal particles makes the flame shape much more intriguing. Specifically, the linear and cubic dust concentration distributions lead to the formation of an asymmetric flame front, due to a higher concentration of the combustible coal particles in the lower half of the channel. Acceleration is strong in the lower branch in all directions so that it catches the upper segment later on. The snapshots of the flame evaluation show that the trough formation and loss of symmetry of the flame front is originated in the region close to the flame cusp.

Finally, let us discuss the effect of a parabolic dust concentration distribution. As one may remember, in this case, the dense combustible particles are distributed through the center of the channel while their concentration decreases towards the upper and lower sidewalls. After ignition of the fuel mixture, an intrinsically unstable flame front tries to generate a trough as observed for the homogeneous distribution. However, the dust particles at the centerline, promote the flame velocity, locally, and thereby prevent a through formation. In other words, the parabolic distribution of the combustible particles stabilizes an intrinsically instable flame front. Consequently, the increase in the flame surface area appears slower, thereby moderating flame acceleration as compared to other distributions considered.

4 Summary

In the present paper, we have investigated flame propagation in a combined gaseous-dusty environment with non-uniform coal dust concentration distributions by means of the computational simulations. It is shown that a non-uniform dust distribution may result in an extra distortion or local stabilization of the flame front, which respectively increases or decreases the total surface area of the flame front, thereby promoting or moderating the flame acceleration scenario. In a future study, we aim to investigate the later stages of flame acceleration due to wall friction that may provide other significant remarks. Moreover, the effect of the particle radius, concentration and different distribution functions can also be examined in a set of parametric simulations. It would also be interesting to investigate the effect of inert particles and their distributions. While the reader may expect some validation of the provided computational platform, unfortunately, we are not aware of any experimental studies and hope that the present study will provide a good platform for more elaborated experiments for combustion of non-uniformly distributed coal particles in a gaseous mixture. Consequently, we believe that this study provides a considerable physical insight not only for the understanding of accidental coalmine flames but also for applications associated with the controlling combustion strategies.

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