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# Computational Study of Premixed Flame Propagation in a Gaseous-Dusty Environment with Various Dust Distributions

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Abstract: Propagation of a gaseous-dusty premixed flame front in a channel, resembling a methane-air fire scenario in a coalmine, is studied by means of the computational simulations. The core of the computational platform is a finite-volume, Navier-Stokes code solving for the reacting flow equations with a fully-compressible hydrodynamics and an Arrhenius chemical kinetics. The combustible coal dust particles are incorporated into the solver by means of the Seshadri formulation such that a real gaseous-dusty environment is replaced by an "effective fluid" with locallymodified, dust-induced flow and flame parameters. The originality of this work is in the consideration of various spatial dust concentration distributions such as the homogenous, linear, cubic and parabolic ones. Specifically, flame acceleration due to wall friction is analyzed for all these distributions; the similarity and differences in the evolutions of the flame morphology and velocity in each of these cases as well as in the case of purely gaseous combustion are identified. It is shown that a non-uniform dust distribution may result in an extra distortion or a local stabilization of the flame front, which respectively increases or reduces the total flame surface area, thereby promoting or moderating flame acceleration. Overall, the effects of non-uniform dust distribution become substantial when the channel width exceeds a certain critical value proportional to the flame thickness.

Keywords: flame acceleration; gaseous-dusty combustion; computational simulation; coalmine fire safety

## 1. Introduction

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

While a planar premixed flame front would propagate steadily, with a certain speed  $S_L$  with respect to the unburnt gas, such a flame occurs rarely in the practical reality. Indeed, the majority of industrial and laboratory flames are usually corrugated due to wall friction, in-built obstacles, turbulence, acoustics, shocks, combustion instabilities, etc. A corrugated flame front has a larger surface area relative to a planar one; therefore, it consumes more fuel per unit time and releases more heat, thus propagating faster than a planar flame front in the same mixture. Consequently, the continuous increase in the flame surface area is accompanied by flame acceleration.

One of the well-known mechanisms of flame acceleration is that by Shelkin [1], devoted to wall friction. Specifically, when a premixed flame propagates in a tube/channel/tunnel with one end open, from the closed end to the open one, it generates a new volume through gas expansion in the burning process and thereby drives a flow in the unburnt gas. Wall friction makes this flow non-uniform, thereby bending the flame front and increasing its surface area. The latter, in turn, promotes the flame velocity and, as a result, the flame-generated flow. Such a positive feedback between the flame and the flow provides flame acceleration. Based on this mechanism, Bychkov *et al.* have developed an analytical theory substantiated by extensive computational simulations [2]. However, the theory and modelling [2] employed a number of simplifications, including the conventional approach of the constant thermal-chemical flame properties such as the unstretched laminar flame speed  $S_L$ . However,  $S_L$  may experience spatial and temporal variations in reality, in particular, due to the combustible (coal) and/or inert (rock) dust impurities within a coalmine.

The present study initiates a systematic investigation of the influence of local variations of the thermal-chemical flame and fuel properties on the global flame dynamics and morphology. This particular work focuses on the effects of  $S_L$ -variations on flame acceleration due to wall friction in a gaseous-dusty premixture. Specifically, the computational simulations of the reacting flow equations, with a fully-compressible hydrodynamics and an Arrhenius chemistry are performed, with the combustible coal dust particles incorporated into the original (gaseous) computational platform by means of the Seshadri formulation [3]. Namely, a real gaseous-dusty environment is replaced by an "effective fluid" with locally-modified, dust-induced flow and flame parameters. Keeping in mind a coalmine passage, we considered flame propagation in a channel with a large aspect ratio. Various spatial distributions of the coal dust concentration are studied, namely: (a) homogenous, (b) linear, (c) cubic and (d) parabolic. While a homogenous dust distribution simply provides a scaling factor as compared to purely gaseous combustion [2], the non-uniform distributions were anticipated to provide qualitatively new features.

As a result, the similarity and differences in the evolutions of the flame shape and velocity have been identified for each distribution. It is shown that the non-uniform distributions may result in an extra distortion or a local stabilization of the flame front, which promotes or reduces the flame surface area, thereby facilitating or moderating flame acceleration due to wall friction.

### 2. Description of the Computational Simulations

The core of the computational platform consists of a fully-compressible, finite-volume Navier-Stokes code solving for the hydrodynamics and combustion equations in gaseous environment. The basic equations read:

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

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

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

where Y is the mass fraction of the fuel mixture;  $\varepsilon = QY + C_V T$  and  $h = QY + C_P T$  are the specific internal energy and enthalpy; Q is the energy release in the reaction;  $C_V$  and  $C_P$  are respectively the specific heats at constant volume and pressure. We consider a single irreversible

reaction of the first-order, of the Arrhenius type, with the activation energy  $E_a$  and the constant of time dimension  $\tau_R$ . The stress tensor  $\gamma_{i,i}$  and the energy diffusion vector  $q_i$  are given by

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

where  $\zeta \equiv \rho v$  is the dynamic viscosity, and Pr and Sc are the Prandtl and Schmidt numbers. We took  $\zeta = 1.7 \times 10^{-5} kg/(m \cdot s)$  and Pr = 1, with the Lewis number being Le = Pr/Sc = 1.0753.

Combustible dust particles have been implemented into this solver by employing the Seshadri formulation [3] that expresses the laminar burning velocity,  $S_{d,L}$ , as a function of local thermalchemical properties of the gas and coal dust in the form

$$S_{d,L} = \frac{1}{Ze} \sqrt{\frac{2Bk_u}{\rho_u C_T}} \exp\left(-\frac{E_a}{R_u T_f}\right), \quad Ze = \frac{E_a (T_f - T_u)}{R_u T_f^2}, \quad C_T = C_P + C_s n_s \frac{4\pi r_s^3}{3} \frac{\rho_s}{\rho}, \quad (5)$$

where Ze is the Zel'dovich number,  $C_T$  is the entire specific heat of the mixture, and  $C_s$  is that of dust particles. Here  $\rho = \rho_u + c_s$  is the density of the mixture, with the density of the fresh gas  $\rho_u$  and the concentration of particles  $c_s$ . 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. Thus the growth of the equivalence ratio promotes the flame temperature  $(T_f^*)$  and, thereby, its propagation velocity  $(S_{d,L}^*)$ ; see Refs. [3, 4] for details.

We utilized this modified computational platform to study the impact of various combustible dust concentration distributions on the scenario of flame acceleration induced by wall friction. In fact, the coal dust distribution is usually non-uniform in a coalmine [5]. A steady 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. Over time, the shock weakens but the shock-heated air is ignited by the lifted dust [5]. Hence, a secondary combustion process is initiated in the premixture made of the gaseous fuel and non-uniformly distributed dust. In this respect, a lifted dust layer may resemble a linear, cubic, or even parabolic distribution due to different energy levels of complex magnetic forces. This example may justify our choice of dust distributions, specified below, though it is difficult to identify the real distribution in a coalmine.



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

The four coal dust concentration distributions used in this work are presented in Fig. 1. First, we employed a uniform distribution, Fig. 1a, which provided a base model for the computational platform. Subsequently, we used three non-uniform distributions along the channel as functions of a radial coordinate. For the linear distribution, Fig. 1b, the maximal concentration,  $c_{s,max}$ , is attained at the bottom of the channel, with no dust at the top. Applying the boundary conditions on the linear gradient of non-uniform dust distribution, we have

$$c_s = c_{s,\max} \left( 1 - x / 2R \right). \tag{6}$$

We also considered a cubic coal dust concentration distribution,

$$c_s = c_{s,\max} \left[ 1 - \left( \frac{x}{2R} \right)^3 \right], \tag{7}$$

as illustrated in Fig. 1c. Finally, we employed a parabolic distribution,

$$c_{s} = c_{s,\max} \left[ 1 - 4 \left( (x - R) / 2R \right)^{2} \right],$$
(8)

depicted in Fig. 1d, where the dust concentration is maximal along the centerline and is zero along the bottom and top of the channel. With x = 0, all Eqs. (6) – (8) obviously yield  $c_s = c_{s,max}$ .

In this work, we modelled lean ( $\phi = 0.7$ ) methane/air/coal dust combustion, which is relevant to the practical reality. In addition, a small particle radius is employed,  $r_s = 10 \mu m$ , with the dust concentration of 120 g/m<sup>3</sup>, which provides an effective equivalence ratio promotion due to a fast pyrolysis. The laminar flame speed for the given equivalence ratio,  $\phi = 0.7$ , in the absence of the dust particles, was taken as  $S_L = 0.169m/s$ , which provided realistically slow, strongly subsonic flame propagation  $S_L << c_0$ , with the flame Mach number  $Ma \equiv S_L/c_o \approx 5 \times 10^{-4}$ . In fact, this fame velocity is reproduced by Eq. (5) with  $c_s = 0$  or  $r_s = 0$ . We took the standard initial fuel pressure, 1 bar, and temperature, 300 K. Thermal expansion in the burning process is determined by the energy release in the reaction and is defined as the density ratio of fuel to burnt matter,  $\Theta = \rho_u / \rho_b$ ; we took  $\Theta = 6.1$  related to methane/air/coal burning at  $\phi = 0.7$  [6]. The gas-phase mixture was modelled as an ideal gas of a constant molecular weight,  $2.9 \times 10^{-2} kg/mol$ . The channel half-width is characterized, conventionally, by the flame propagation Reynolds number,  $\operatorname{Re}_f = RS_{L,mean} / v = R / \operatorname{Pr}L_f$ , where  $L_f \equiv v / \operatorname{Pr}S_L = 8.65 \times 10^{-5}m$  is the thermal flame thickness.

#### 3. Result and Discussion

Figure 2 compares the characteristics of the accelerating flames for different dust distributions. Specifically, Fig. 2a shows the velocity of the flame position at the centerline,  $U_c$ , scaled by  $S_L$ , versus the scaled time,  $\tau = t S_{L,mean} / R$ . First of all, we observe that the parabolic dust distribution moderates flame acceleration as compared to a homogeneous case. However, the most important observation is a sudden jump of the flame velocity, around  $\tau \sim 0.25$ , for the linear and cubic distributions. Indeed, the flame velocity grows almost by an order of magnitude for methane-airdust combustion; such a rise might even lead to a detonation for much faster flames, such as hydrogen-oxygen ones [2]. Also, the plots for the linear and cubic distributions closely resemble each other. We also studied the case of no dust, which showed similarity with the homogeneous distribution. Figure 2b presents the evolution of the scaled flame front surface area,  $A_w / 2R$ . The growth of the flame surface area promotes its velocity. In the case of a parabolic distribution, the lower flame surface area mitigates flame acceleration as depicted in Fig. 2a.



Figure 2: The scaled flame velocity  $U_c/S_L$  (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: Color temperature snapshots at the instants  $\tau = 0.15$  (a), 0.27 (b), 0.36 (c) and 0.61 (d)

What mechanism is responsible for such a trend? To answer this question, we investigated the evolution of the flame shape for all distributions at identical time instants 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 its closed end to the open one. Subsequently, the flame front gets corrugated due to wall friction generating non-uniform flow velocity field. For the homogeneous distribution, we observe formation of a trough, which gets stronger with time. Later, the central segment of the flame accelerates faster than the upper and lower ones; see also Fig. 2a. At the end, only a small through is visible. The origin of the trough may be attributed to the Darrieus-Landau combustion instability allowable by the considered  $\text{Re}_f = 24$  [2]. It is noted that a non-

uniform distribution of dust particles makes the shape of the flame front much more intriguing. Specifically, the linear and cubic distributions lead to the formation of an asymmetric flame front, due to a higher concentration of the combustible particles in a lower half of the channel. Acceleration is strong in the lower branch in all directions so that it catches the upper part later on. The snapshots of the flame evaluation show that the trough formation and a loss of symmetry of the flame front is originated in the region close to the flame cusp.

Finally, we discuss the effect of the parabolic dust concentration distribution. After ignition of the fuel mixture, an intrinsically unstable flame front tries to generate a trough. However, the dust particles located at the centerline promote the flame velocity, locally, and thereby prevent such a through formation. In other words, the parabolic dust concentration distribution stabilizes an intrinsically instable flame front. Consequently, the increase in the flame surface area appears slower, thereby moderating flame acceleration as compared to the other distributions considered.

## 4. Summary

The present work scrutinizes flame propagation in a combined gaseous-dusty environment with non-uniform coal dust distributions by means of the computational simulations. It is shown that a non-uniform dust distribution may result in either an extra distortions or a local stabilizations of the flame front, which increases or decreases the total flame front surface area, respectively, thereby promoting or moderating flame acceleration. Consequently, it is believed that this study is actual not only for the preventive strategies against accidental coalmine fires, but is also for the general development of the controlling combustion strategies in various applications.

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# 6. References

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