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Ignition of deflagration and detonation ahead of the flame due to radiative preheating of suspended micro particles

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ABSTRACT

We study a flame propagating in the gaseous combustible mixture with suspended inert solid micro particles. The gaseous mixture is assumed to be transparent for thermal radiation emitted by the hot combustion products, while particles absorb and reemit the radiation. Thermal radiation heats the particles, which in turn transfer the heat to the surrounding unburned gaseous mixture by means of thermal heat transfer, so that the gas phase temperature lags that of the particles. We consider different scenarios depending on the spatial distribution of the particles, their size and the number density. In the case of uniform spatial distribution of the particles the radiation causes a modest increase of the temperature ahead of the flame and corresponding modest increase of the combustion velocity. In the case of non-uniform distribution of the particles (layered dust cloud), such that the particles number density is relatively small in the region just ahead of the flame front and increases in the distant regions ahead of the flame, the preheating caused by the thermal radiation may trigger additional independent source of ignition. Far ahead of the flame, where number density of particles increases forming a dense cloud of particles, the radiative preheating results in the formation of a temperature gradient with the maximum temperature sufficient for ignition. Depending on the steepness of the temperature gradient formed in the unburned mixture, either deflagration or detonation can be initiated via the Zel'dovich's gradient mechanism. The ignition and the resulting combustion regimes depend on the number density profile and, correspondingly, on the temperature profile (temperature gradient), which is formed in effect of radiation absorption and gas-dynamic expansion. The effect of radiation preheating as stronger as smaller is the normal flame velocity. The effect of radiation heat transfer in the case of coal dust flames propagating in layered particle-gas deposits cloud can result in the spread of combustion wave with velocity up to 1000 m/s and it is a plausible explanation of the origin of dust explosion in coal mines.

1. Introduction

It is known that uncontrolled development of detonation poses significant threats to chemical storage and processing facilities, mining operations, etc. [1,2], while controlled detonation initiation can be a potential application for propulsion and power devices [3]. In astrophysics type Ia supernovae (SNe Ia) were used as a standard distance indicators and led to the one of the most impressive discovery of the accelerating expansion of the universe [4–6]. However, the nature of thermonuclear explosion of SN Ia and specifically the mechanism of transition to detonation during the thermonuclear explosion of SN Ia still remains the least understood aspect of the thermonuclear supernovae explosion phenomenon [7–11].

While studying combustion in gaseous mixture, the radiation of hot combustion products is not taken into account, as the radiation absorption length in a gaseous mixture is very large, so that the gaseous mixture is almost fully transparent for the radiation and therefore the radiation heat transfer does not influence the flame dynamics. The situation changes drastically in the presence of particulates of size r_p suspended in the gaseous mixture, which is typical for e.g., coal mine, chemical industry, forest fire, etc. In such a case the absorption length of radiation can be estimated as $L = 1/N_p\sigma_p$, where N_p is the particles number density, and $\sigma_p = \pi r_p^2$ is the particles cross section for the light absorption. The radiant energy flux is absorbed by the particles and then lost by conduction from the particles surface to the surrounding unreacted gaseous phase so that the gas phase temperature lags that of the particles. It should also be noted that even the presence of a relatively small concentration of particles increases the luminosity considerably, so that the radiant flux emitted by the hot combustion products may be well approximated by the black-body radiation. Particles preheated by the absorbed radiation

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increase temperature of the surrounding unburned gaseous mixture affecting the flame dynamics. Studies of the premixed flames and detonations arising and propagating in the presence of suspended particulates may play an important role for the understanding of unconfined vapor cloud explosions, accidental explosions in the coal mines and in the chemical industry, dust explosion hazards, and for better performance of rocket engines using the solid fuels. In the present paper we show that the radiative preheating may not only affect the flame structure, increase the velocity of the propagating flame, but also can trigger a new source of ignition of either deflagration or detonation in the unburned mixture ahead of the flame front.

A combustible mixture can be ignited by electrical sparks, or by thermal heating. The ignition capability of an electrical spark varies with fuel concentration, humidity, oxygen content of the atmosphere, temperature, and turbulence, requiring about 0.01/0.03 mJ depending on the mixture reactivity. In contrast, radiation-induced ignition typically requires much larger amounts of energy to be released in the mixture. Direct thermal ignition of gaseous combustible mixture by absorption of radiation causing a rapid increase in temperature at least up to 1000 K is possible by focusing a high power laser radiation and has been demonstrated both theoretically and experimentally [12,13]. However, ignition at low power levels is unlikely because of a very large length of absorption of the combustible gases at normal conditions.

The flame propagating in the uniformly dispersed, quiescent, gravity-free, particle clouds and radiation affected combustion in the presence of inert particles has been studied by different groups of authors assuming uniform dispersion of particulates with and without account of radiative heat transfer [14–22]. The dynamics of particle-laden flames affected by the radiative preheating has been studied in [14–16] using asymptotic methods and a one-step Arrhenius chemical model with high activation energy. Coal combustion research [22,23] is typically focused on two aspects of practical interest: production of volatiles due to thermal decomposition of coal dust and char combustion. For the coal-dust suspension in air filling the coal-fired burners and rocket engines using the solid fuels as well as for coal-fire mining safety problems both the ignition and combustion evolution are of paramount importance [22,23]. The combustible volatiles may essentially contribute to the heat-up of the coal particles, enhance the combustion energy release due to energy feedback mechanism resulting in an explosion. Effect of the radiation heat transfer on a spray combustion, which can be of interest for practical cases such as diesel engines, gas turbine combustors etc. was studied in [24].

In practice, the plausibility of ignition is determined by the ignition conditions implying certain energy input with a certain rate. As the mechanism formulated above involves suspended particles as a carrier of radiation energy and since particles have to be heated up to relatively high temperature, their spatial distribution should be such, that the radiation will be absorbed mostly far ahead of the flame front in order to promote the ignition conditions before the flame arrival. Ignition may occur via the Zel'dovich temperature gradient mechanism [25] with initiating of one or another combustion regime depending on the gradient steepness. The thermal energy accumulated by the particles and transferred to the gaseous mixture depends on the radiant energy absorbed by the particles, the energy transferred from the particle surface to surrounding gaseous mixture and the radiant loss from the particles.

In the present paper we consider the effects of thermal radiative preheating using as an representative example a flame propagating in the suspension comprising two phases: hydrogen oxygen gaseous mixture and inert solid micro particles. The hydrogen oxygen gaseous mixture is assumed to be transparent for radiation, while the solid particles absorb and reemit the radiation. We consider different scenarios depending on spatial distribution of the suspended particles ahead of the propagating flame. For a uniform spatial distribution of suspended particles in the gaseous mixture the radiative preheating of the particles ahead of the flame results in the increase of the gaseous mixture temperature and correspondingly in the increase of the combustion wave velocity. All the same the effect of radiation is noticeably stronger for the particle-dust flames with a small normal velocity, for example, for methane-air coal dust flames. On the contrary, a non-uniform spatial distribution of dispersed particles, such that the concentration of particles is smaller in immediate proximity ahead the flame and increases ahead of the flame forming a denser cloud of particles suspended in the gaseous mixture, may result in ignition of either deflagration or detonation via the Zel'dovich gradient mechanism. In the case of coal dust flames propagating through the layered particle-gas cloud the effect of radiation heat transfer can result in the spread of combustion wave with velocity up to 1000 m/s and presumably explain the origin of dust explosion in coal mines.

The paper is organized as follows. Section 2 is the formulation of the problem and short description of the numerical method. In Section 3 we perform 1D direct numerical simulations and consider the planar hydrogen–oxygen flame propagating through the mixture with uniform distribution of small suspended particles. Section 4 presents analysis of the ignition of different combustion regimes initiated by the radiative preheating in the case of non-uniform distribution of dispersed particles. We conclude in Section 5. Details of the numerical scheme used in simulations together with thorough convergence and resolution tests are presented in Appendices A and B.

2. Governing equations

The governing equations for a planar flame in the gaseous phase are the one-dimensional, time-dependent, multispecies reactive Navier–Stokes equations including the effects of compressibility, molecular diffusion, thermal conduction, viscosity, chemical kinetics and the chemical energy release, momentum and heat transfer between the particles and the gas:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \tag{1}$$

$$\frac{\partial Y_i}{\partial t} + u\frac{\partial Y_i}{\partial x} = \frac{1}{\rho}\frac{\partial}{\partial x}\left(\rho D_i \frac{\partial Y_i}{\partial x}\right) + \left(\frac{\partial Y_i}{\partial t}\right)_{\mathrm{ch}}, \tag{2}$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}\right) = -\frac{\partial P}{\partial x} + \frac{\partial \sigma_{xx}}{\partial x} - \rho_{\mathrm{p}}\frac{(u-u_{\mathrm{p}})}{\tau_{\mathrm{St}}}, \tag{3}$$

$$\begin{aligned}\rho\left(\frac{\partial E}{\partial t} + u\frac{\partial E}{\partial x}\right) &= -\frac{\partial Pu}{\partial x} + \frac{\partial}{\partial x}(\sigma_{xx}u) + \frac{\partial}{\partial x}\left(\kappa(T)\frac{\partial T}{\partial x}\right)\\ &+ \sum_k h_k\left(\frac{\partial}{\partial x}\left(\rho D_k(T)\frac{\partial Y_k}{\partial x}\right)\right) + \rho\sum_k h_k\left(\frac{\partial Y_i}{\partial t}\right)_{\mathrm{ch}}\\ &- \rho_{\mathrm{p}}u_{\mathrm{p}}\frac{(u-u_{\mathrm{p}})}{\tau_{\mathrm{St}}} - \rho_{\mathrm{p}}c_{\mathrm{p,p}}Q,\end{aligned} \tag{4}$$

$$P = R_{\mathrm{B}}Tn = \left(\sum_i \frac{R_{\mathrm{B}}}{m_i}Y_i\right)\rho T = \rho T\sum_i R_i Y_i, \tag{5}$$

$$\varepsilon = c_v T + \sum_k \frac{h_k \rho_k}{\rho} = c_v T + \sum_k h_k Y_k, \tag{6}$$

$$\sigma_{xx} = \frac{4}{3}\mu\left(\frac{\partial u}{\partial x}\right) \tag{7}$$

We use here the standard notations: P, ρ, u, are pressure, mass density, and flow velocity of gaseous mixture, $Y_i = \rho_i/\rho$ is the mass fractions of the species, $E = \varepsilon + u^2/2$ is the total energy density, ε is the