

Influence of Radiative Preheating on Flame Propagation in Gaseous Mixtures Seeded with Inert Particles

M.A. Liberman¹ M.F Ivanov², A. D. Kiverin,²

¹ Nordita, KTH Royal Institute of Technology and Stockholm University
Stockholm, Sweden

² Joint Institute for High Temperatures of RAS
Moscow, Russia

1 Introduction

Usually radiation of hot combustion products is not important for a flame dynamics, inasmuch as the unburned gaseous fuel is almost fully transparent for the radiation. The situation changes drastically in the presence of particulates suspended in the gaseous mixture, which is typical for e.g., coal mine, chemical industry, forest fire, etc. In these cases, for example for coal dust-air flames, the radiant heat flux is absorbed by the particles so that the radiation influences the flame propagation, and the radiation heat transfer may even be the dominant mechanism of energy transfer. The absorbed thermal radiation heats the particles and they transfer the heat to the surrounding unburned gaseous mixture affecting the flame dynamics. There are different scenarios of the radiative preheating in the presence of suspended micro particles depending on mixture reactivity and correspondingly the flame velocity and the value of radiation absorption length. The result of radiative preheating can be a modest increase of the temperature ahead of the fast flame and corresponding modest increase of the combustion velocity, or noticeable increase and oscillation of the flame velocity for slow flames. It is shown that non-uniform spatial distribution of temperature caused by the radiative preheating results in the ignition of either deflagration or detonation ahead of the flame front via the Zeldovich's gradient mechanism. In the present study the effects of thermal radiative preheating is considered for the flames propagating in the suspension comprising two phases: gaseous mixture (H_2/O_2 or H_2/air) and inert solid micro particles. The gaseous mixture is assumed to be transparent for radiation, while the particles absorb and reemit the radiation.

2 Governing Equations

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 gaseous phase were solved numerically for a planar flame propagating in a channel filled with the stoichiometric H_2/O_2 mixture with suspended micro particles. The standard reduced chemical kinetic scheme for hydrogen/oxygen combustion [1] was used in simulations. The equations for gaseous phase are:

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

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

$$\rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) = -\frac{\partial P}{\partial x} + \frac{\partial \sigma_{xx}}{\partial x} - \rho_p \frac{(u - u_p)}{\tau_{St}}, \quad (3)$$

$$\rho \left(\frac{\partial E}{\partial t} + u \frac{\partial E}{\partial x} \right) = -\frac{\partial Pu}{\partial x} + \frac{\partial}{\partial x} (\sigma_{xx} u) + \frac{\partial}{\partial x} \left(\kappa(T) \frac{\partial T}{\partial x} \right) + \sum_k h_k \left(\frac{\partial}{\partial x} \left(\rho D_k(T) \frac{\partial Y_k}{\partial x} \right) \right) + \rho \sum_k h_k \left(\frac{\partial Y_k}{\partial t} \right)_{ch} - \rho_p \frac{(u - u_p)^2}{\tau_{St}} - \rho_p c_{P,p} Q_{gp}, \quad (4)$$

The equations for the phase of suspended particles read:

$$\frac{\partial N_p}{\partial t} + \frac{\partial(N_p u_p)}{\partial x} = \frac{\partial}{\partial x} \left(D_m \frac{\partial N_p}{\partial x} \right), \quad (5)$$

$$\left(\frac{\partial u_p}{\partial t} + u_p \frac{\partial u_p}{\partial x} \right) = \frac{(u - u_p)}{\tau_{St}}, \quad (6)$$

$$\left(\frac{\partial T_p}{\partial t} + u_p \frac{\partial T_p}{\partial x} \right) = Q_{gp} - \frac{2\pi r_p^2 N_p}{c_{P,p} \rho_{p0}} (4\sigma T_p^4 - q_{rad}), \quad (7)$$

Here we use the standard notations: P , ρ , u , u_p are pressure, mass density, and velocities of gaseous phase and particles, $Y_i = \rho_i / \rho$ - the mass fractions of the species, $E = \varepsilon + u^2 / 2$ - the total energy density, ε - the internal energy density, R_B - is the universal gas constant, m_i - the molar mass of i-species, $R_i = R_B / m_i$, n - the gaseous molar density, $c_v = \sum c_{vi} Y_i$ - is the constant volume specific heat, $\kappa(T)$ and $\mu(T)$ are the coefficients of thermal conductivity and viscosity, $D_i(T)$ - is the diffusion coefficients of i-species, $(\partial Y_i / \partial t)_{ch}$ - is the variation of i-species concentration (mass fraction) in chemical reactions. T_p , N_p are temperature and particles number density, $\rho_p = m_p N_p$, $\tau_{St} = m_p / 6\pi\mu r_p$ is the Stokes time for the spherical particles of the radius r_p , $D_m = kT_g / 6\pi\mu r_p$ is the coefficient of molecular (Brownian) diffusion. The thermal energy transferred from the particle surface to the surrounding gaseous mixture is

$$Q_{gp} = (T - T_p) / \tau_{gp} = \frac{3\kappa Nu}{2r_p^2 c_{P,p} \rho_{p0}} (T - T_p), \quad (8)$$

where $\tau_{gp} = 2r_p^2 c_{P,p} \rho_{p0} / 3\kappa Nu$ is the characteristic time of the energy transfer, Nu is the Nusselt number. The thermal radiation heat transfer in the diffusion approximation is [2, 3]:

$$\frac{d}{dx} \left(\frac{1}{\chi} \frac{dq_{rad}}{dx} \right) = -3\chi (4\sigma T_p^4 - q_{rad}), \quad (9)$$

$\chi = 1/l = \pi r_p^2 N_p$ and $l = 1/\pi r_p^2 N_p$ are the radiation absorption coefficient and the radiation absorption length. Region of the combustion products behind the flame front is assumed optically thick, so that the radiation energy flux emitted from the flame front is close to the blackbody radiation, $q_{rad}(x = X_f) = \sigma T_b^4$, where σ is the Stefan-Boltzmann constant, and $T_b = 3000\text{K}$ is the adiabatic temperature of the hot combustion products. In all the calculations the mass loading parameter, $\varsigma = m_p N_p / \rho$, was taken small so that there is only one-way coupling, i.e., particles do not affect the gaseous flow. In this case the initial temperatures and the initial flame velocities are the same and therefore it allows to distinguish the effects of the radiation preheating.

3 Effects of Radiative Preheating on Combustion Regimes

The calculations were carried out for stoichiometric hydrogen/oxygen at initial pressure $P_0 = 1\text{atm}$ using the standard reduced chemical kinetic scheme for hydrogen/oxygen combustion [4]. Detailed description of the numerical method and transport coefficients was presented in [5, 6]. The thorough convergence and resolution tests were carried out to verify that the observed phenomena are remaining unchanged with increasing resolution. The acceptable resolution of at least 48 computational cells per width of the flame was used for quantitative convergence.

Figure 1 shows (left part) the calculated gaseous and particles temperature profiles, and the corresponding increase of the combustion velocities (right) for different radiation absorption lengths, $\ell = 0.28, 1.11, 2.22\text{ cm}$ ($r_p = 6; 1.5; 0.75\mu\text{m}$, $N_p = 3.18 \times 10^6; 1.27 \times 10^7; 2.55 \times 10^7\text{ cm}^{-3}$) in case of the initial uniform particles distribution.

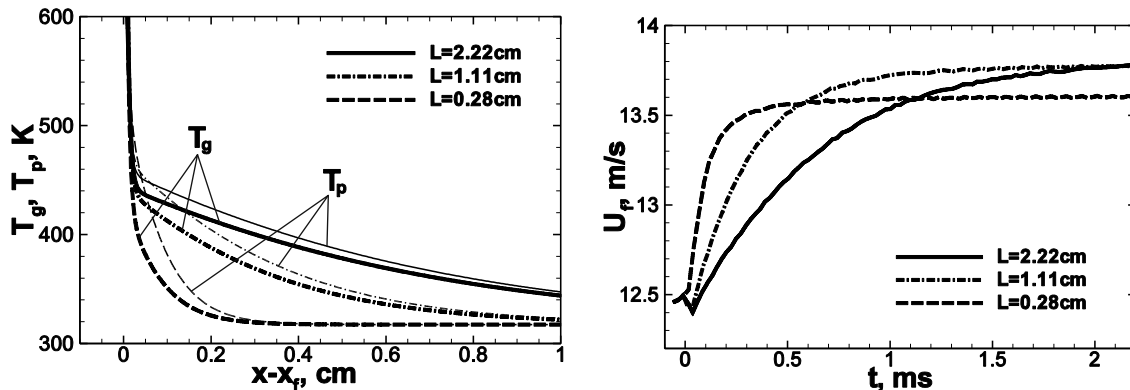


Figure 1. Left: Temperature profiles ahead of the flame front calculated for uniformly distributed suspended particles: $\ell = 0.28, 1.11, 2.22\text{ cm}$. Right: The corresponding increase of the burning velocity.

The flame velocity increases due to heating of the particles which absorbed the radiant flux and heat the surrounding unburned mixture ahead of the flame ($\Delta T \approx 150 \div 200\text{K}$). As shorter the absorption length is as shorter the preheated zone ahead of the flame and as faster the flame velocity increases. It should be noticed that the characteristic time of the energy transfer from the particles to surrounding gaseous mixture, τ_{pg} , is of the order of the characteristic gas-dynamic time $t_h = L_f / U_f$. This limits the maximal temperature of the gas phase for a fast flames because the flame consumes the nearest higher temperature parts of the mixture before its temperature achieved its equilibrium value. Taking into account that a stationary flow is formed during the time of the order $1 / U_f$ it is straightforward to obtain an order-of-magnitude estimate of temperature increase within the radiation absorption length. The maximum temperature increase of the particles in the layer of width δ close to the flame front is $\Delta T_p \approx 3\sigma T_b^4 \delta / 4r_p \rho_p c_p U_f$. One can readily observe that the maximum temperature of the particles

preheated by radiation from the H_2/O_2 flame corresponding to conditions of Fig.1 is $\Delta T \approx (120 \div 130)K$ for $\ell = 1.1cm$ in agreement with the calculated temperature increase in Fig.1. For the same conditions but in case of H_2/air flame instead of H_2/O_2 flame, and taking into account that in this case $T_b = 2100K$, maximum temperature ahead of the flame front during the radiative heating is $\Delta T \approx 200K$ for $\ell = 1.1cm$. For the slow normal velocity flame, for example methane/air, the radiative preheating can rise temperature within the absorption length up to the value, which is enough for the ignition. In the latter case the radiative heat transfer competes with the gaseous diffusion and thermal conduction and can become a dominant one as the mechanism of the combustion wave propagation. In such a case the combustion wave propagates due to the sequential ignitions in the region of radiation absorption length ahead of the flame front and the width of the flame is of the order of the radiation absorption length. For a laminar flame propagating as a result of thermal conduction, it is straightforward to obtain an order-of-magnitude estimates for the width and speed of the flame using a dimensional analysis: $L_{fg} \propto \sqrt{\chi \tau_R}$ and $U_{fg} \propto \sqrt{\chi / \tau_R}$, where $\chi = \kappa_g / \rho c_{g,p}$, and τ_R is the characteristic reaction time. An order-of-magnitude estimate for the width and speed of the combustion wave in the case, when the radiative heat transfer dominates, is $U_{f_{rad}} \propto 1 / \tau_R \approx (1 / L_{fg}) U_{fg}$, which is considerably larger than the normal laminar velocity of the flame in a pure gaseous mixture.

If velocity of a laminar flame is small enough the maximum temperature achieved within the radiation absorption length can exceed the value required for the ignition, and the formed temperature gradient can ignite either deflagration or detonation via the Zel'dovich gradient mechanism. Since the space scale of such gradient for a detonation ignition in case of slow reactive mixtures is quite large, about meter or larger [7, 8], so that large computational resources are required for the numerical modeling, we illustrate the phenomena for H_2/O_2 gaseous mixture with non-uniform space distribution of the micron size particles as it is shown schematically in Fig.2. The particle number density ahead of the flame is such that the mixture is transparent for the radiation and the particle number density increases further away from the flame in a denser cloud with a steep or diffuse left boundary.

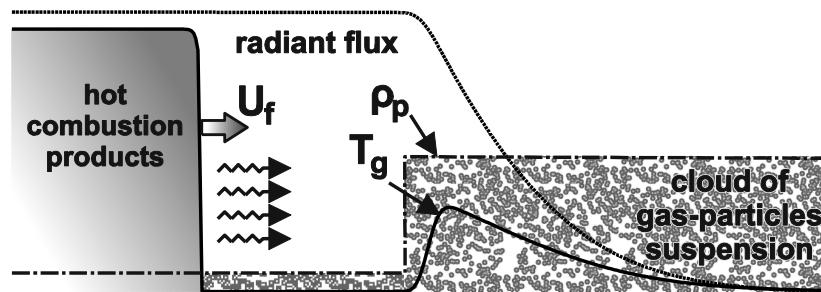


Figure 2: Radiant preheating of the gaseous mixture inside the gas-particles cloud far ahead the flame front.

Particles in the dense cloud far ahead from the flame absorb the thermal radiant energy flux so that temperature of the surrounding gaseous mixture rises up to the value suitable for ignition before the flame arrives to the cloud. The crossover temperature for H_2/O_2 where the induction endothermic stage passes into the fast exothermic stage is $1050 \pm 50K$. The temperature non-uniformity originating due to the radiative preheating in the gas-particle cloud via radiation absorbed by the particles depends on the radiation absorption length, the local gas density and the gas expansion during the heating.

Depending on the steepness of the formed temperature gradient, either a deflagration or a detonation can be ignited via the Zeldovich's gradient mechanism. The calculated temperature gradient, $\Delta = (T^* - T_0) / |dT / dx| \approx 1cm$, for the initial stepwise profile of particles number density, $r_p = 1\mu m$, $N_p = 2.5 \cdot 10^7 cm^{-3}$, is close to the radiation absorption length $l = 1 / \pi r_p^2 N_p \approx 1.2cm$ and it results in initiation of a deflagration via the Zeldovich's gradient mechanism.

Figure 3 shows the results of the simulation for the cloud of particles with initial diffuse left boundary, where the particles number density drops linearly on the scale of 10cm from the maximum particles number density $N_p = 2.5 \cdot 10^7 \text{ cm}^{-3}$. Dashed line at the upper frame shows the initial linear density profile. Solid line corresponds to the density profile at time instant prior to the ignition, which was smeared due to gas expansion during the thermal radiation heating up to 20cm at the time instant $t_0 = 4980 \mu\text{s}$ prior to the ignition of a spontaneous combustion wave triggering the detonation. Temporal evolution of the gaseous temperature and pressure profiles during the detonation formation in the vicinity of the diffusive cloud boundary are depicted in the two other frames.

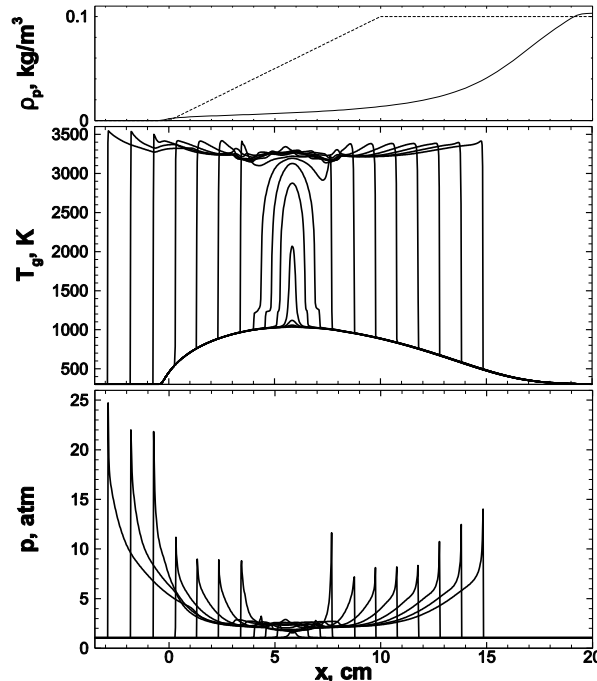


Figure 3. The detonation formation in the vicinity of the diffuse boundary of gas-particles cloud far ahead the propagating flame front. The upper frame shows the distribution of particles mass density: dashed line – the initial linear density profile of width 10.0cm, solid line – density profile at time instant prior to the ignition.

4 Conclusion

The present study indicates that the radiative preheating in the presence of a gas-particle heat exchange considerably influences the overall picture of the flame propagation. Depending on the value of the normal laminar flame velocity in the pure gaseous mixture and on the spatial distribution of the particles number density, the radiative preheating can either result in the increase of the flame velocity, or can promote formation of the temperature gradient, which can ignite either deflagration or detonation via the Zeldovich's gradient mechanism ahead of the flame front. The performed numerical simulations demonstrate the plausibility of radiation preheating as the principal effect of the combustion intensification or a detonation initiation in the gaseous fuel, where relatively low concentration of suspended solid particles or some other substance can absorb the radiative heat flux and rise temperature of the fuel ahead of the flame. It should be emphasized that this study is a necessary prerequisite aiming to show principle physics and role of the radiative preheating. The obtained results show that the thermal radiative preheating can play a significant role in determining the regimes of combustion in two-phase reacting flows. The conditions under which a reactive two-phase mixture can ignite and produce a heat release are also considered to be important in the area of fire safety. It should be noticed that in case of a slow reactive mixture and correspondingly much slower flames, such as methane-air flame, the radiative preheating results in much stronger increase of

the flame velocity compared to that shown in Fig.1 for H₂/O₂. In particular, small oscillations of the flame velocity, seen in the right part of Fig.1, will be much more pronounced. There was indication that for coal dust-air flames the radiation could be the dominant mechanism of energy transfer and the flame propagation.

References

- [1] Zeldovich YaB. (1980) Regime Classification of an Exothermic Reaction with Nonuniform Initial Conditions. *Combust. Flame*, 39: 211.
- [2] Zeldovich YaB, Raizer Yu. (1966) *Physics of Shock waves and High-Temperature Hydrodynamic Phenomena*, Academic Press.
- [3] Siegel R, Howell JR. (1993) *Thermal Radiation Heat Transfer*, 3ed Edition, Taylor & Francis Group.
- [4] Warnatz J, Maas U, Dibble RW. (2001) *Combustion. Physical and chemical fundamentals, modeling and simulations, experiments, pollutant formation*, Springer.
- [5] Lieberman MA, Eriksson L-E, Ivanov MF, Piel OD (2005) Numerical Modeling of the Propagating Flame and Knock Occurrence in Spark-Ignition Engines. *Combust. Sci. and Tech.* 177: 151.
- [6] Ivanov MF, Kiverin AD, Lieberman MA (2011) Flame acceleration and DDT of hydrogen-oxygen gaseous mixtures in channels with no-slip walls. *Int. J. Hydrogen Energy*, 36: 7714.
- [7] Lieberman MA, Kiverin AD, Ivanov MF (2011) On Detonation Initiation by a Temperature Gradient for a Detailed Chemical Reaction Models. *Phys. Letters A* 375: 1803-1808.
- [8] Lieberman MA, Kiverin AD, Ivanov MF (2012) Regimes of chemical reaction waves initiated by nonuniform initial conditions for detailed chemical reaction models. *Phys.Rev.* E85: 056312.