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On the formation of new ignition kernels in the chemically active dispersed mixtures

M F Ivanov and A D Kiverin

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

E-mail: ivanov_mf@mail.ru

Abstract. The specific features of the combustion waves propagating through the channels filled with chemically active gaseous mixture and non-uniformly suspended micro particles are studied numerically. It is shown that the heat radiated by the hot products, absorbed by the micro particles and then transferred to the environmental fresh mixture can be the source of new ignition kernels in the regions of particles' clusters. Herewith the spatial distribution of the particles determines the features of combustion regimes arising in these kernels. One can highlight the multi-kernel ignition in the polydisperse mixtures and ignition of the combustion regimes with shocks and detonation formation in the mixtures with pronounced gradients of microparticles concentration.

1. Introduction

The contemporary problems of heterogeneous (or two-phase) combustion and explosion arise first in association with assessments of fire and explosion safety of a wide class of industrial objects (coalmines, chemical industry plants, nuclear plants). In case of gaseous combustible mixtures for today such problems, become traditional with enough clear understanding of the leading factors defining ignition and combustion evolution. The situation changes, becoming more complicated when studying the heterogeneous mixtures comprising inert or chemically active microparticles. Further, we will consider only mixtures with suspended inert microparticles. It is obvious that in general case the suspended inert microparticles would reduce intensity of all the combustion phases beginning from the ignition and until the detonation formation, even causing the quenching of the combustion. On the other hand, the particles ahead of the propagating flame front absorb the radiant heat emitted from the hot combustion products and then transfer it to the environmental fresh mixture. Such a mechanism of mixture preheating promotes combustion intensification. Meanwhile the role of radiant heat transfer is one of the less studied aspects of heterogeneous combustion.

One knows that the gas at normal density is transparent for the radiant heat (the free path length of the radiation is about hundreds of meters in order of magnitude). On the other hand, the presence of the absorbing particles reduces drastically the radiation free path length. Qualitatively the competition between mentioned above factors of flow deceleration and radiant mixture preheating was studied in analytical works [1, 2] and references within. Based on simplified models the authors studied the combustion of the reacting gas densely seeded with small particles. Recently in [3] we studied numerically the scenarios of flame propagation

through hydrogen-oxygen mixture seeded with microparticles. It was shown that in case of mixture uniformly seeded with microparticles the radiant preheating could not cause more than 10 percent increase of the burning velocity. Otherwise, in case of non-uniformly suspended microparticles the preheating of the distant particles cloud could result in a formation of new ignition kernels changing sufficiently the combustion pattern.

The aim of the present paper was to study in details the role of absorbing radiant heat in a formation of autoignition kernels far ahead of the propagating flame front. We considered problems of autoignition in monodisperse and bidisperse mixtures with spatially non-uniform distribution of the particles.

2. Problem setup

We consider a planar one-dimensional flow generated due to the flame propagation through the channel from its closed end (the left bound of the computational domain). At the initial time instant the channel is filled with stoichiometric hydrogen-oxygen mixture at normal conditions ($p_0 = 1.0$ atm and $T_0 = 300$ K), the microparticles of size $d_p = 1.5$ μm are distributed in a way that in the region of primal ignition their concentration is small (close to zero) while at the distance of L_0 from the ignition zone the concentration rises up to the finite value $N_p = 6 \times 10^7$ cm^{-3}. Schematically the problem setup is presented in figure 1.

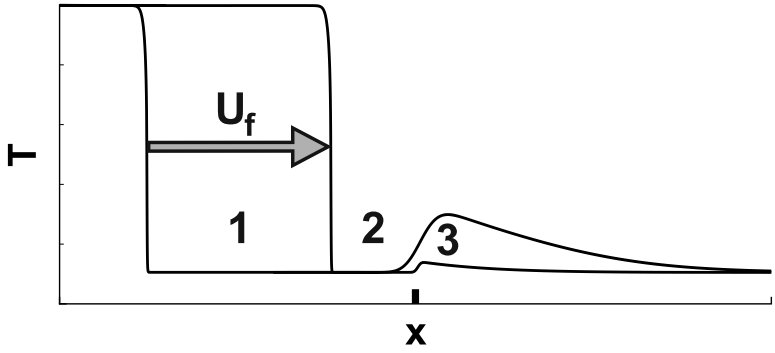

Figure 1. Schematic representation of the problem setup in the coordinates referred to the particles cloud margin. 1—combustion products region, 2—the gap between the flame front and the cloud margin, 3—heating region.

Dynamics of the chemically active gaseous mixture is described by the Navier-Stokes equations for viscous compressible medium including thermal conductivity, multicomponent diffusivity, energy and momentum exchange with suspended microparticles and energy release inside the reaction zone. The system of equations has a standard form, presented e.g. in [4, 5]. Coefficients of viscosity, thermal conduction and diffusivity for gaseous phase are calculated according to the relations from kinetic theory for multicomponent gaseous mixtures [6]. Equations of state for fresh combustible mixture and combustion products are calculated using the interpolation of NASA tables [7]. The system of gasdynamics equations is solved using the euler-lagrange algorithm [8] modified and approved in [4, 5] and our previous papers. To reproduce features of chemical reaction of combustion we implemented the reduced kinetic mechanism for hydrogen combustion from [6]. The stiff system of reaction kinetics differential equations were solved using the Gear method from the standard mathematical library SLATEC. The phase of suspended microparticles is modeled as a continuum [9] that allows us to use gasdynamic-like equations to determine the dynamics of the particles

$$\frac{\partial N_p}{\partial t} + \frac{\partial N_p u_p}{\partial x} = 0, \tag{1}$$

$$\frac{\partial u_p}{\partial t} + u_p \frac{\partial u_p}{\partial x} = F_{St}, \tag{2}$$

$$\frac{\partial T_p}{\partial t} + u_p \frac{\partial T_p}{\partial x} = Q_{gp} - \frac{\pi r_p^2 N_p}{c_{P,p}\rho_{p0}}\Big(4\sigma T_p^4 - q_{rad}\Big), \tag{3}$$

where N_p—particles number density, u_p—particles velocity, T_p—particles temperature, r_p—particle radius, $c_{P,p}$—specific heat capacity of the particles material, ρ_{p0} density of the particles material.

The interaction of the two phases and momentum exchange are implemented in the energy and momentum equations in a form of a Stokes force term

$$F_{St} = \frac{6\pi r_p \mu}{m_p}\Big(u - u_p\Big) \tag{4}$$

with characteristic relaxation time calculated as

$$\tau_{St} = \frac{m_p}{6\pi r_p \mu}, \tag{5}$$

where m_p—particle mass, μ—molecular dynamical viscosity of the gas and u_g—gas mass velocity.

The thermal exchange is described by the empirical law expressing the thermal flow via the Nusselt number [10]

$$Q_{gp} = \frac{3\kappa Nu}{2r_p^2 c_{P,p}\rho_{p0}}\Big(T_g - T_p\Big), \tag{6}$$

where T_g—gas temperature, κ—gas thermal conductivity. The characteristic time of inter-phase heat exchange is calculated as

$$\tau_Q = \frac{2r_p^2 c_{P,p}\rho_{p0}}{3\kappa Nu}. \tag{7}$$

The momentum and heat exchange between phases should be also implemented in the equations for gaseous phase. The momentum balance equation should be supplemented with term $-\rho_p F_{St}$, the energy equation should be supplemented with terms $-\rho_p u_p F_{St} - \rho_p c_{P,p} Q_{gp}$, where $\rho_p = m_p N_p$—mass density of the disperse phase.

The last term in equation 3 determines the radiant heat absorption by the particles. q_{rad} is a radiant heat flux, $4\sigma T_p^4$ is a flux emitted from the particle surface, σ–Stefan–Boltzmann constant. Radiation transfer is calculated in the diffusion approximation that adequately describes the features of the radiation transfer through heterogeneous medium, its absorption on the particles surface and reradiation from their surface. The diffusive equation for radiant flux q_{rad} is

$$\frac{d}{dx}\Big(L\frac{q_{rad}}{dx}\Big) = -\frac{3}{L}(4\sigma T_p^4 - q_{rad}), \tag{8}$$

where L—free path length of radiation, calculated as $L = (\pi r_p^2 N_p)^{-1}$, where r_p and N_p are particles radius and concentration correspondingly.

In the poly-disperse mixtures containing the particles of different sizes comparable with the wavelength of the transferred radiation the radiation transfer is described in a multi-group approximation. The particles of different sizes absorb only the part of the spectrum with wavelengths shorter than the characteristic length scale of the absorption (particle diameter). In such a case in a mixture containing particles of sizes r_{pi} ($r_{p,i+1} > r_{pi}$) one can distinguish groups corresponding to the ranges of wave lengths $\Delta\lambda_i = \{2r_{p,i-1} < \lambda < 2r_{pi}\}$ (r_{pN} is a radius of a larger particle, r_{p1} is a radius of a smaller particle, $r_{p0} = 0$). The equation 8 should be replaced by the system of N equations for partial radiant fluxes $q_{rad,i}$ absorbing only in the

range of wave lengths $\Lambda_i = \{0 < \lambda < 2r_{pi}\}$. Further, in calculations for bidisperse mixtures we will use two-group approximation:

$$\begin{cases} \frac{d}{dx}\left(L\frac{q_{rad,2}}{dx}\right) = -\frac{3}{L}\int_{r_{p1}}^{r_{p2}} cU_{\lambda,p}d\lambda + \frac{3}{L_2}q_{rad,2}, \\ \frac{d}{dx}\left(L\frac{q_{rad,1}}{dx}\right) = -\frac{3}{L}\left(\int_{0}^{r_{p1}} cU_{\lambda,p}d\lambda - q_{rad,1}\right), \end{cases} \tag{9}$$

where the local radiation path length is calculated taking into account the presence of the particles of two types limiting it with the smallest value of L_i—$L = L_1L_2/(L_1 + L_2)$.

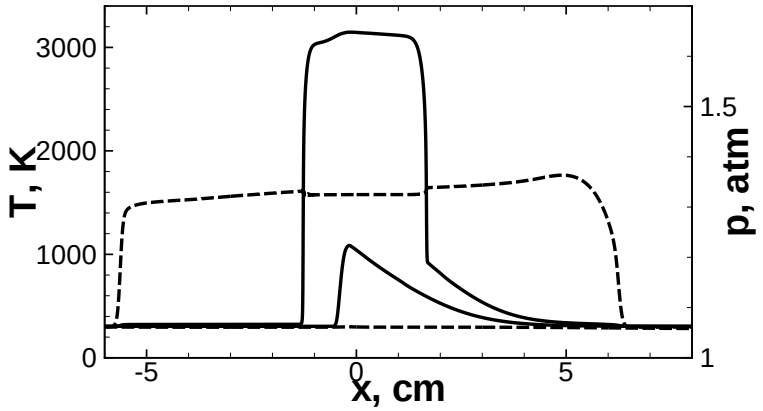

Figure 2. Temperature (solid lines) and pressure (dashed lines) profiles at different time instant corresponding to the pre-ignition phase ($t_0 = 0.9$ ms) and combustion phase ($t = 1.0$ ms) in the monodisperse mixture with non-uniformly distributed microparticles ($N_p(x) = N_p\eta(x)$).

3. Results and discussion

3.1. Mechanism of radiant preheating

As the planar flame propagates through the channel from its closed end the expansion of the combustion products trigger the flow, accelerating the fresh mixture and the propagating flame front. The initially static fresh mixture accelerates up to the velocity $u_f = (\Theta - 1)U_f$ while the flame front in the laboratory reference frame accelerates up to the $U_{f,L} = \Theta U_f$, where U_f is a burning velocity and $\Theta = \rho_f/\rho_b$ is an expansion factor determined as a ratio of fresh mixture and burning products densities. According to this the flame consumes the moving combustible mixture with a relative velocity equal to burning velocity U_f. Therefore the flame should reach the margin of the moving distant cloud during $\Delta t = L_0/U_f$. The criterion of the successful autoignition at the particles cloud margin can be formulated as follows. If the time of the gas-particle mixture heating up to the characteristic ignition temperature is shorter than the time of flame arrival to the particles cloud margin, the independent ignition will occur. For the following parameters of the particles $d_p = 1.5\mu m$, $\rho_{p,0} = 1.0$ g/cm^3, $c_{P,p} = 10^7$ erg/g/K, their distribution $N_p = 6 \times 10^7$ cm^{-3} and radiant flux emitted from the flame front $q_{rad} = \sigma T_p^4 = 4.6 \times 10^9$ erg/s/cm^2 (where combustion products temperature is $T_b = 3000$ K) the time of hydrogen-oxygen mixture heating up to the characteristic ignition temperature of 1050 K can be estimated as $\Delta t = 1.0$ ms by the order of magnitude. Thus the minimal distance L_0 between the cloud margin and primal ignition zone should be not less than 1.0 cm for successful autoignition ($U_f = 1200$ cm/s).

Let us consider an ignition kernel formation at the margin of the particles cloud in case when the initial particles distribution has a step-wise distribution ($N_p(x) = N_p\eta(x)$, where $x = 0$ is a

cloud margin position). Particles heated by the absorbed radiant flux transfer the heat to the environmental gas causing its expansion and corresponding redistribution of the particles inside the absorption region. As a result, one can observe a non-uniform temperature distribution with local maximum at the clouds boundary and descending temperature gradient inside the cloud. As the characteristic time scales of radiant heating and inter-phase thermal exchange is much larger than acoustic time scale the pressure inside the absorption zone equalizes and the ignition takes place at almost constant pressure equal to the initial one. The ignition takes place via the mechanism of non-steady thermal explosion in the presence of temperature gradient first proposed by Ya B Zel'dovich [11]. As one can see in figure 2, the ignition at the step-wise margin causes the formation of slow combustion wave propagating out from the cloud margin.

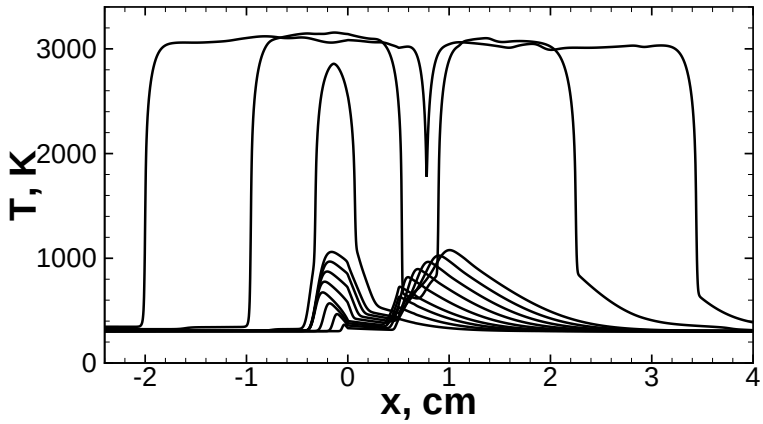

Figure 3. Temperature profiles at sequential time instants representing the heated kernels formation and further ignition in polydisperse mixture with non-uniform particles distribution ($N_{p1}(x) = N_{p1}\eta(x) - N_{p1}\eta(x-l)$, $N_{p2}(x) = N_{p2}\eta(x-l)$). $t_0 = 50$ μs, $\Delta t = 100$ μs.

3.2. Multi-kernel ignition in the polydisperse medium

Now let us consider the features of ignition kernels formation in the medium seeded with particles of different sizes (polydisperse medium). Let us analyze the particles distribution such that the radiant flux will first overcome a thin layer (of width $l = 0.5$ cm) of small particles with radiation free path length L_1 and then propagate through the medium with radiation free path length L_2 seeded with larger particles ($N_{p1}(x) = N_{p1}\eta(x) - N_{p1}\eta(x-l)$, $N_{p2}(x) = N_{p2}\eta(x-l)$). According to such a problem setup the thin layer absorbs the radiation in the range of wave lengths $\lambda < d_{p1}$. In the remaining space ($x > l$) the waves with $\lambda < d_{p2}$ are absorbed on the free path length L_2 (d_{p1} and d_{p2} are the particles diameters, $d_{p1} < d_{p2}$). To simplify the analysis the parameters of the particles are chosen in a way to avoid the distinctions in their dynamics and features of inter-phase thermal exchange. Figure 3 represents the evolution of the temperature distribution inside the absorption zone. One can observe a formation of "two-humped" temperature profile due to the changes in absorption mechanisms first on the margin between gas and thin layer of small particles and then on the margin between this layer and the region seeded with larger particles. The ignition occurs independently in both kernels. Thus in the polydisperse medium the regime of multi-kernel ignition becomes possible. It determines higher intensity of the combustion and as a result higher intensity of dynamic loads that is of interest for explosion safety problems.

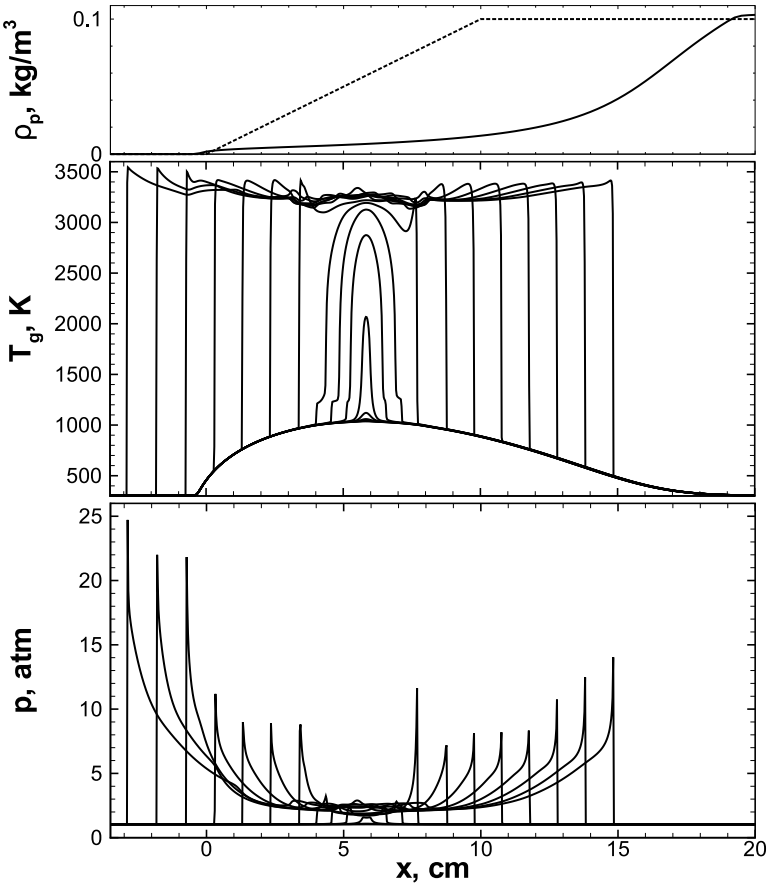

Figure 4. Temperature (middle) and pressure (bottom) profiles at sequential time instants representing the detonation formation inside the absorption zone ($N_p(x > 0) = N_p x/h$). The upper domain shows the particles redistribution during the pre-ignition phase. $t_0 = 4.98$ ms, $\Delta t = 4$ μs.

3.3. Shock waves and detonation formation at the smooth cloud margin

As it was mentioned above the ignition inside the absorption zone arises via the Zel'dovich gradient mechanism [11]. In cases presented above (see figures 2, 3) the heat absorption on the step-wise margins causes relatively small smoothening of the margin and correspondingly rather steep temperature gradient formation. According to the Zel'dovich classification such a steep gradient corresponds to the ignition of slow combustion wave (see also [12]). However if it becomes possible to achieve more smooth temperature distribution the fast combustion waves with shocks running ahead or even detonation waves will arise.

In real situation in presence of convective flows, there should be no step-wise margins between pure gas and gas-particles clouds. The margins are diffusively smoothening in the space and the absorption inside such regions with non-uniform particles distribution causes formation of distinct temperature profiles. We carried out the calculations with initial non-uniform distribution of the particles $N_p(x > 0) = N_p x/h$, where h is a thickness of the initial cloud margin. It can be shown that as initial rate of margin's smoothening (h) rises the temperature gradient in the vicinity of its maximum becomes shallower and more violent combustion regimes can arise. The slow combustion transforms into the fast combustion propagating behind the outrunning shock wave and then into the detonation. The latter case of detonation formation

inside the autoignition kernel is represented in figure 4. In natural conditions the probability of such an autoignition regimes point out the high explosiveness of combustible heterogeneous mediums.

4. Conclusions

The numerical results allowed us to demonstrate hazardous specific features of combustion inside the chemically active heterogeneous mixtures with non-uniform distribution of inert microparticles. In presence of evolving flame front the local clusters (clouds) of microparticles distant from the primal ignition zone absorbs the radiant heat emitted from the hot combustion products. If the distance between the cloud margin and the primal ignition zone is large enough the radiant heating can cause local auto-ignition far ahead of the propagating flame. The independent ignitions intensify the combustion sufficiently. In case of polydisperse mixture, the probability of multi-kernel ignition arises. In presence of spatial gradients of particles' concentration, the shallow temperature gradients arise that in turn leads to the formation of fast combustion waves, shock waves and even detonation. The discussed results on heterogeneous combustion and explosion regimes triggered by radiant transfer and absorption allow estimate the explosiveness of chemically active dispersed media.

Acknowledgments

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