Direct initiation of gaseous detonation via radiative heating of microparticles volumetrically suspended in the gas

V P Efremov, M F Ivanov, A D Kiverin and I S Yakovenko
Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
E-mail: alexeykiverin@gmail.com

Abstract. We propose a new conceptual approach for direct detonation initiation in the gaseous mixtures seeded with micro particles via the radiative heating from the external energy source. The basic mechanisms of energy absorption, ignition and detonation formation are analyzed numerically on the example of hydrogen-oxygen mixture. Obtained data is very promising and allows us to formulate conditions for the source power to ignite detonation in certain system geometry.

1. Introduction

Energy effective regimes of gaseous fuels combustion are of considerable interest nowadays. In propulsion systems design it is prospective to use detonative regime [1] instead of classic deflagration (slow combustion) regime. Commonly one considers two basic approaches of detonation initiation: direct initiation and deflagration-to-detonation transition (DDT). On the one hand, in the latter case the amount of energy required to ignite detonation is less than in the first case. On the other hand, DDT is not well reproducible. Its probability strongly depends on the chemical composition, thermodynamic state of the mixture and geometry of the combustor. Moreover in number of cases including the most practically interesting gaseous fuel-air mixtures flame acceleration provides only trans- or supersonic flame instead of detonation [2]. Such combustion regimes provide less effective thermodynamic cycle compared to detonative one. As opposed to DDT the direct detonation initiation is more accurately controllable technique. Principally to predict the resulting combustion regime one should know only the evolution of energy deposition (energy amount, source power and spatial localization) [3]. Main drawback of such an approach is the requirement for high-power sources. High intensity action on the gaseous mixture generates essential dynamic loads on the combustor’s shell.

In number of cases (especially when the spatially localized onset of detonation is required), it can be perspective to use contactless approach that provide mild ignition of detonation via the volumetric explosion. In paper [4] it is proposed to use single walled carbon nanotubes as a carrier of excess energy. Nanotubes’ restructuring and evaporation under the thermal radiation cause local internal energy release sufficient to ignite detonation in the surrounding gas. The process of radiative heating of the gaseous combustible mixture seeded with microparticles formally can be splitted into two basic stages. First stage is gas heating via the interphase heat transfer...
from the particles surface. Second one is the heat release from the burning particles. Today the information on the second phase is not enough for quantitative estimations as there are still discrepancies in reaction rates and heat effects for nanotubes decomposition. However, it can be shown that in cases of sufficient intensity of radiation source or long enough action time the combustible mixture ignition can be achieved already on the first stage even in mixtures where suspended particles have large activation energies or are completely inactive [5]. In practice, high intensity of thermal radiation can be achieved by using the coherent sources of energy.

Because of the abovementioned facts, the concept of direct detonation initiation on the fixed spatial-time scales can be elaborated. The aim of this paper was to substantiate the conceptual approach of localized direct detonation initiation via the radiative heating of the suspended microparticles. We consider possible scenarios of ignition kernels evolution and detonation onset in the localized volume of gaseous combustible mixture with suspended inactive microparticles under effect of the external radiative energy source. Sensitivity of the developing combustion regime towards particles spatial distribution and energy source intensity is studied. It allows us to formulate criteria for proposed concept applicability. The analysis is carried out by means of numerical simulations for one of the simplest gaseous combustible mixtures of hydrogen with oxygen. Oxy-fuel mixtures have relatively low energy threshold of detonation initiation and by themselves can be considered as a perspective detonator for air-fuel mixtures.

2. Problem setup
Assume the following problem setup. Consider the channel filled with stoichiometric hydrogen-oxygen mixture at normal conditions (300.0 K and 1.0 bar). The layer of thickness $L_1$ carries uniformly suspended inactive microparticles. The suspended particles parameters are following: diameter $d_p = 1.0\ \mu m$, material density $\rho_p = 1.0\ \text{g/cm}^3$, specific heat capacity $c_{p,p} = 10^7\ \text{erg/g/K}$, volume fraction of the particles $\alpha_p = 1.0 \times 10^{-5}$–$4.0 \times 10^{-5}$. At this setup the mean free path length of the radiation inside the layer can be estimated as $L = 6.7–1.7\ \text{cm}$ ($L = 2d_p/3\alpha_p$, taking into account that the gaseous phase is almost transparent for radiation). It is assumed that constant radiative heat flux is instantly switched on at time $t = 0$. Parameters of the radiative energy source are the same as in [4]. The emitted heat flux $q_s = \sigma T^4$ correspond to the black body surface with temperature of $5800.0\ \text{K}$. In most of calculations, the duration of the source action was not limited, however it was found that radiation did not influence the detonation after its formation. Thus, the obtained results also can be considered as the estimation of minimal radiative pulse duration required to ignite detonation.

Numerical simulations were carried out using thoroughly tested reactive gasdynamics codes for calculating planar and multidimensional reactive flows (see e.g. authors papers [3, 5]). Used one-dimensional gasdynamic model is two-temperature, two-velocity and is based on Navier–Stokes equations for compressible viscous medium involving thermal conductivity, multicomponent diffusion and chemical transformation according to the reduced kinetic mechanism from [6]. The phase of suspended microparticles was considered by using continual approximation. The interphase exchange of momentum and energy was calculated using the Stokes law. During the radiative heating inactive particles did not change their size and phase state. This assumption is quite acceptable as temperature is lower than $1050.0–1100.0\ \text{K}$ on the stage prior to the ignition. Afterwards the energy balance is changing mainly by the exothermal reaction of combustion and the phase transitions play almost no role in further evolution of combustion. Radiative heat transfer was calculated according to the diffusive approximation. Combustion products remained transparent for the radiation. For more complete description of the mathematical model for two-phase reactive gasdynamics and the numerical algorithm one can address to the recent paper [5].
Figure 1. Evolution pattern of the detonation initiation inside heated gas-particles layer of 1.5cm initial thickness, $L = 3.33$ cm. Color shows mass density of the particles phase. Lines show temperature isolines of 1500 K (dashed) and 3000 K (solid). Frame (a) shows both stages of radiative heating and detonation formation, (b) represents enlarged region of ignition and detonation formation. 1—far margin of the layer, 2—first ignition point, 3—region of energy release in the nonstationary thermal explosion, 4—region of compression behind the outrunning shock, 5—point of detonation onset, 6—detonation wave locus in the cold fresh fuel.

3. Results and discussion
The heating of the gaseous mixture is determined by radiative heat absorption on the particles’ surfaces and by further heat transfer from these surfaces to the surrounding gas. The rate of uniformity of gas heating is fully determined by the volume fraction and spatial distribution of the particles. During the heating process, gaseous mixture expands in both directions carrying microparticles away from the heated region. As a result, the local concentration of the particles decreases. Further heating continues in the non-uniform medium with larger mean free path. If the particles layer thickness is large such that rarefaction waves have no time to disturb medium inside the layer before the ignition the temperature distribution will reproduce the profile of radiative flux decreasing exponentially with the depth ($T(x) \sim \exp(-x/L)$). In case of thin layer, the heating is almost uniform as the rarefaction equalizes its non-uniformity. Figure 1a represents characteristic pattern of the process evolution including the stage of heating and expansion and the stage of detonation initiation. The data are presented for the thin layer of $L_1 < L$ where the heated medium expands almost symmetric on the first stage. The detonation arises inside the heated layer and propagates into the cold fresh fuel (in figure 1a the locus of the self-sustained detonation is shown by isotherm of 3000.0 K). Figure 1b represents more details of ignition and detonation onset that will be discussed below.

In the studied range of particles volume fractions the heating time up to the ignition is longer than the acoustic time scales ($t_{\text{ign}} > L/c$, where $c$—local sonic speed). Therefore, the ignition
Figure 2. Calculated criteria of transition between different mechanisms of detonation formation. (1) \(L_{\text{min}}\) — minimal particles layer thickness sufficient for detonation formation (dash-dotted line), (2) \(L_{\text{1max}}\) — maximum particles layer thickness providing detonation formation as a result of thermal explosion evolution (solid line), (3) \(L_{\text{max}}\) — particles layer thickness providing detonation formation (dashed line).

arises inside the non-uniformly heated kernel at almost constant pressure. Ignition regimes in such a case correspond to non-stationary thermal explosion solution derived by Ya B Zel’dovich for the ignition on the temperature gradient [7]. Figure 2 shows zones of considered scenarios of detonation formation depending on the layer thickness \((L_1)\) and initial mean free path of radiation \((L)\). The detonation arises only in the region between curves 1 and 3. In the region below curve 2 the detonation arises in full accordance to the non-stationary thermal explosion solution. In the region above this curve, the sufficient role in detonation formation belongs to the secondary shock waves re-reflected from the layer boundaries.

Let us consider the regimes of ignition and combustion evolution inside the layers of different initial thickness. In case of thin layer a smooth temperature distribution forms and a so-called “weak detonation” arises. Reaction wave propagates via series of independent ignitions (as a so-called spontaneous wave) along temperature gradient with visible speed equal to \(|\text{grad}(\tau_{\text{ind}})|^{-1}\) (sufficiently high in case of smooth gradient, as \(\tau_{\text{ind}}\) is induction period that decreases with temperature rise). As the visible speed is supersonic, a compression wave follows the reaction front. Propagating along the temperature gradient the reaction front decelerates and couples with the compression wave that results in detonation formation. However, in case of thin layer the heated volume can be not enough for complete evolution of the process and “weak detonation” will enter the cold fresh fuel, that will be not sufficient to ignite self-sustained detonation. Therefore, a criterion on minimal layer thickness \(L_{\text{min}}\) exists (curve 1 on figure 2) below which no self-sustained detonation formation is possible. As the layer thickness increase the temperature gradient inside the layer becomes steeper (asymptotically approaching \(\sim \exp(-x/L)\) distribution). In case of steeper temperature gradient, the deceleration of spontaneous wave causes its degeneration into the combustion wave. In turn, the compression wave overruns reaction front forming a shock wave. In figure 1b, the zone of energy release in the non-stationary thermal explosion (propagating in a form of spontaneous wave) is marked with ‘3’ while the compression zone behind the outrunning shock wave is marked with ‘4’. Figure 1b shows the typical scenario occurring with the increase of layer thickness. The reaction front accelerates as it consumes the compressed fuel and transforms into the detonation wave (point ‘5’). The mechanism of transient detonation formation is close to that arising in deflagration-to-detonation transition [8] and immediately after the transition detonation wave propagates...
Figure 3. Ignition time (dashed line) and first ignition point position relative to the initial layer’s margin (solid line) dependence on heat radiation flux.

in the “overdriven” regime (see also the “SWACER” solution for near-limit direct detonation initiation via spark plug [9]). Overdriven detonation carries higher pressure and temperature and is able to ignite self-sustained detonation in the cold fresh fuel. With further increase in the layer thickness, the formed complex of shock wave followed by the reaction front is unable to initiate detonation and only a fast deflagration wave can be formed. However, one more rather unobvious scenario of detonation formation can be observed. Shock wave reflects from the contact surface at the far margin of the layer and propagates backwards interacting with the reaction front. The interaction of reaction front with the shock re-reflected from the near margin is also possible. Additional transfer of the momentum and energy by re-reflected shocks causes reaction front acceleration with sequential transition to detonation. This mechanism of transition to detonation due to the shock-to-reaction interaction (region between curves 2 and 3 in figure 2) is rather sensitive towards external conditions and should be classified as unstable scenario. Finally, a layer thickness $L_{\text{max}}$ exists which provides weak rarefaction, formation of steep temperature gradient and as a result conditions for shock attenuation and no detonation formation on the scales of gas-particles layer. Summing up, it occurs to be possible to ignite self-sustained detonation inside the layers of the thickness between certain limits.

Figure 3 illustrates the influence of energy source’ power on the process evolution. Curves in figure 3 show the position of the first ignition point (solid) and corresponding ignition time (dashed) as they depend on the energy flux normalized to the one discussed above ($q_s$). Duration of the heating up to the ignition temperature decreases exponentially with rising source intensity. At first sight, this fact might increase the stability of the formulated approach. Furthermore, as source intensity is raised the first ignition point tends to shift towards the initial position of the near layer margin that provides high rate of detonation origin localization. However, one should take into account that the temperature equilibrium between radiatively heated particles and gas establishes only during the finite time $\tau_Q$, determined by the relaxation of the gaseous temperature to the particles temperature and by the heat transfer through the gas between neighboring particles. Therefore the temperature equilibrium calculated according to two-temperature model will be possible only if the duration of heating ($t_{\text{ion}}$) is large enough compared with $\tau_Q$. Otherwise, one obtains a system consisting of hot particles suspended inside the cold gas. In such a case ignition arises independently in the vicinity of spatially separated particles that cannot provide conditions for detonation formation as the reaction fronts evolves inside small kernels ($\sim d_p$) and the dissipation can prevent volumetric explosion with necessary parameters. According to its determination the time scale $\tau_Q$ can be estimated
as \( \tau_Q = \frac{k^2}{2} \left( \frac{\rho_p \rho + \rho}{\rho_p \rho_0} + \frac{L_0 \kappa c_{v,g}}{2} \right) \), where \( \kappa \)—molecular thermal conduction of the gas phase, \( Nu \)—Nusselt number, \( \rho_p = \alpha_p \rho_0 \)—mass density of the particles phase, \( \rho \)—gas density, \( c_{v,g} \)—gas specific heat capacity, \( L_0 \)—mean distance between neighboring particles, that can be estimated as \( L_0 = \left( \frac{m_p}{\rho_p} \right)^{1/3} \), \( m_p \)—particle mass. For parameters considered above (case of \( L = 3.33 \text{ cm} \)) time of inter-phase heat transfer \( \sim 0.1 \mu s \) while time of heat redistribution between neighboring particles is about 300–400 \( \mu s \). Therefore the regimes presented in figure 3 below \( q_s = 6 \times q_{s0} \) should correspond to the real temperature distribution and can be reproduced by means of natural experiment with accuracy up to non-uniformities in the spatial distribution of particles and their size distribution.

Consider influence of non-uniformity in particles spatial distribution on the regimes of ignition and detonation formation. Such a distribution was modeled as a system of thin particles layers (\( \sim 0.1–1.0 \text{ cm} \)) separated by layers of pure gaseous mixture. On the stage of radiative heating, the outer layers screen the inner layers diminishing the role of rarefaction. As a result, the heating up to the ignition temperature occurs faster compare with the case of single layer. At the same time, the maximum of the temperature is located in the central part of the system. Here reaction wave evolves not in accordance to the spontaneous mechanism but via combined mechanism involving gasdynamical impact of the already ignited layer on the neighboring one. Shocks emitted out from the ignition kernels transfer momentum and energy triggering faster ignition of the neighboring heated layers. Visible speed of the reaction front increases as well as the shock intensity that finally causes transition to detonation. It should be noted that the position of ignition kernel in the central part could result in detonation formation in two directions away from and towards the energy source.

4. Conclusions

We demonstrated a new concept for controllable (adjusted position and time) direct gaseous detonation initiation via the radiative heating of the inactive microparticles suspended in the combustible mixture.

Conditions of stable detonation initiation were obtained. Influence of source power, gas-particle layer thickness and spatial non-uniformity in particles distribution were considered.

It was shown that non-uniformities in spatial distribution of the particles cause principal change in the regimes of ignition and detonation formation.

Acknowledgments

The study was funded by Russian Science Foundation (grant No. 14-50-00124).

References

[1] Roy G D, Frolov S M, Borisov A A and Netzer D W 2004 J. Progr. Energy Combust. Sci. 30 545
[2] Peraldi O, Knystautas R and Lee J H S 1986 Proc. Combust. Inst. 21 1629
[3] Kiverin A D, Kassoy D R, Ivanov M F and Liberman M A 2013 Phys. Rev. E 87 033015
[4] Finigan D J, Dohm B D, Mockelman J A and Oehlschlaeger M A 2012 Combust. Flame 159 1314
[5] Ivanov M F, Kiverin A D and Liberman M A 2015 Combust. Flame doi:10.1016/j.combustflame.2015.06.018
[6] Warnatz J, Maas U and Dibble R W 2006 Combustion (Berlin: Springer-Verlag)
[7] Zeldovich Ya B 1980 Combust. Flame 39 211
[8] Ivanov M F, Kiverin A D, Liberman M A and Yakovenko I S 2013 Intl. J. Hydrogen Energy 38 36 16427
[9] Bach G G, Knystautas R and Lee J H 1969 Proc. Combust. Inst. 12 853