Mechanisms of Ignition by Transient Energy Deposition: Detailed Chemical Reaction Model

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1 Introduction

Transient thermal energy deposition into a reactive gas provides a source for ignition of either deflagration or detonation. Sufficiently fast and large energy addition can facilitate direct initiation of detonation. Detonation can be initiated by a strong shock (strong explosion) or it can arise as a result of a proper temperature gradient formation through the Zeldovich' mechanism [1]. In most practical cases ignition arises in a small area of combustible mixture which is locally heated by energy input by means of electric spark, hot wire, focused laser light and the like. Such a transient energy addition can generate a wide range of gas expansion processes depending on the amount and the rate of energy actually added and may result in the non-uniform temperature distribution formation. In general case it can be non-uniform distribution of temperature, pressure and/or concentration of reactants which determines ignition and further evolution of the reaction wave through the Zeldovich mechanism. An example of concentration non-uniformity formation is a gas leakage and its distribution by convective flow in the room. In the present work we study mechanisms of chemical reaction wave ignition and regimes of its further propagation in the reactive gaseous mixtures whose chemistry is governed by chain-branching kinetics depending on the characteristics of a transient thermal energy deposition localized in a finite volume of reactive gas. We show that the main parameters which define regimes of the combustion waves facilitated by the transient deposition of thermal energy are: duration of the energy deposition, ignition time scale and acoustic timescale defined by the size of hot spot. The interplay between these parameters specifies the role of gasdynamical processes, the formation and steepness of the temperature gradient and speed of the spontaneous wave. The obtained results give the values of energy and power required for ignition of one or another regime of combustion wave, which is important for the practical use and particularly for risk assessments.

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2 Problem Setup

We consider stoichiometric hydrogen-oxygen mixture at uniform initial conditions (P_0=1atm, T_0=300K) and transient external source of energy localized on the scale of "hot spot" $0 \le x \le L$ where energy Q_{ig} is added during the time Δt_Q. For the sake of simplicity we assume that the rate of the energy addition is linear in time, so that total energy deposition is $Q_{ig} = W\Delta t_Q$, where W is the power of the external source of energy. Gasdynamics of the explosion initiated by the localized energy deposition is characterized by the interrelationship between the time characterizing energy deposition Δt_Q and the characteristic time scales of the problem. The concomitant motion in the gaseous mixture is characterized by acoustic time $t_a = L / a(T)$, where $a(T)$ is the sound speed. The heat from the hot spot propagates in the surrounding gas at the distance $x \sim (4\chi t)^{0.5}$, and the characteristic time of temperature elevation in the surrounding gas is $t_T \sim x^2 / \chi$ [3]. Whether the chemical reaction starts and what processes define the regime of combustion wave depends on the interrelationship between Δt_Q, t_a, t_T and ignition time t_{ign} at the obtained temperature and pressure. Here the ignition time t_{ign} characterizes the length of induction phase after or during the transient energy deposition $t_{ind}(T,P)$. The induction time is measured experimentally and determines local properties of the combustible mixture depending on its thermodynamic state. For the temperature range $T = (1100-1500)\mathrm{K}$, where typically the exothermic reaction starts, the induction time is about ten microseconds (for hydrogen-oxygen). If the reaction started, further heating and energy deposition do not matter and do not affect the formed combustion regime. Thus, of the main interest are the regimes of ignition with $\Delta t_Q < t_{ign}$. For a short time of the energy addition, much less than the acoustic time ($\Delta t_Q << t_a$), mixture in the hot spot can be heated to any temperature and the ignition regime will be determined by the induction time at the obtained temperature and pressure. In case of longer energy deposition the ignition regime will depend on the size of the hot spot (and correspondingly on t_a) and the relation between Δt_Q and t_a. For the hot spots of sizes $L = 1cm$ and $L = 1mm$, the acoustic times are $t_a \approx 20\mu s$ and $t_a \approx 2\mu s$, correspondingly, ($a_0(T = 300K) = 539m/s$).

The governing equations used in the studies are the one-dimensional version of time-dependent, multispecies reactive Navier-Stokes equations including the effects of compressibility, molecular diffusion, thermal conduction, viscosity and chemical kinetics with subsequent chain branching, production of radicals and energy release [2].

3 Rapid energy deposition on microsecond time scale

We consider first the cases when the time scales of the energy deposition and ignition are comparable to or shorter than the characteristic acoustic time scale As it was mentioned above of main interest are the hot spots with $t_a \sim 1-20\mu s$. Thus here we discuss microsecond and submicrosecond timescales of the energy deposition. The submicrosecond energy addition ($\Delta t_Q \le t_{ign} << t_a$) causes almost uniform fast elevation of pressure and temperature inside the energy deposition area (the hot spot) resulting in the volume explosion. The temporal evolution of temperature at the center of the hot spot ($x = 0$) for different values of the added energy is shown in Fig.1 for $\Delta t_Q \sim 0.1\mu s < t_{ign} << t_a$. After the end of the energy deposition and the induction period, reaction starts and then the stationary combustion regimes are established after about 1ms. For each value of deposited energy there is some definite temperature and pressure at which reaction starts and the combustion regime is produced by the volumetric explosion at these conditions.

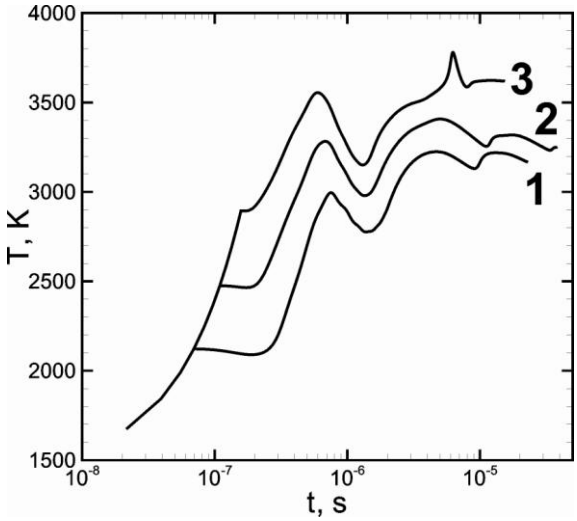
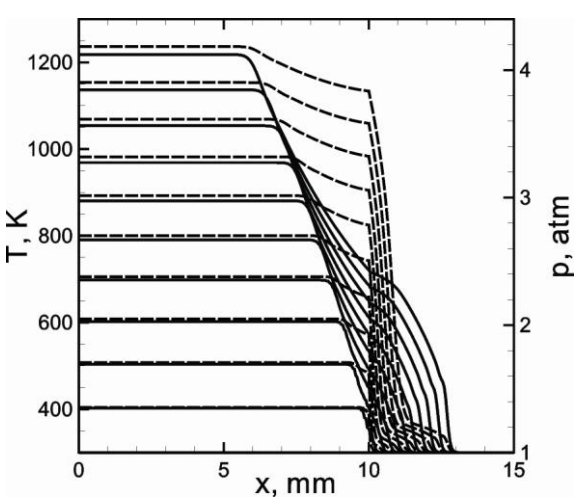


Figure 1. Temperature evolution in the center of the hot spot for $\Delta t_Q = (0.1 \div 0.2)\mu s$; 1 – deflagration ($Q = 1.9 kJ/m^2$), 2 – fast deflagration ($Q = 2.4 kJ/m^2$), 3 - detonation ($Q = 3.0 kJ/m^2$).



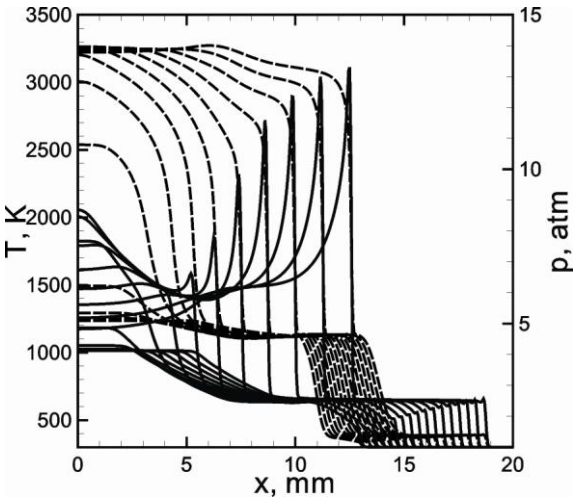


Figure 2(a). Evolution of temperature (dashed lines) and pressure (solid lines) profiles in the hot spot during energy deposition, $L = 1cm$, $\Delta t_Q = 5\mu s$; interval between profiles $\Delta t = 0.5\mu s$.

Figure 2(b) - Evolution of temperature (dashed lines) and pressure (solid lines) profiles illustrating detonation formation in the energy release region, $L = 1cm$, $\Delta t_Q = 5\mu s$;. interval between profiles $\Delta t = 0.5\mu s$.

For less intensive energy deposition ($\Delta t_Q \leq t_{ign} < t_a$) a large pressure jump is forming at the boundary of the hot spot. If power is large enough, subsequent events represent the decay of the discontinuity consisting of a compression wave propagating in the direction $x > 0$, which steepens into the shock wave, and the rarefaction wave propagating to the left from the boundary of hot spot with the velocity equal to the local sound speed. Such scenario can result in the direct triggering of a detonation wave if a concomitant shock wave at the right boundary is strong enough. More interesting scenario emerges in the case of weaker shock and is shown in Figs. 2 (a,b). Fig. 2(a) shows the time evolution of the temperature and pressure profiles inside the hot spot ($L = 1cm$) during the energy deposition. The rarefaction wave propagating to the left creates a shallow temperature and pressure gradients on the scale of about the size of the hot spot. At initial pressure $P_0 = 1atm$ the temperature gradient with the temperature difference and the length scale $L \sim 1cm$ cannot trigger detonation [2]. However, joint temperature and pressure gradient with peak pressure ~4atm can produce a detonation through the Zeldovich gradient mechanism. Corresponding time evolution of the temperature and pressure profiles

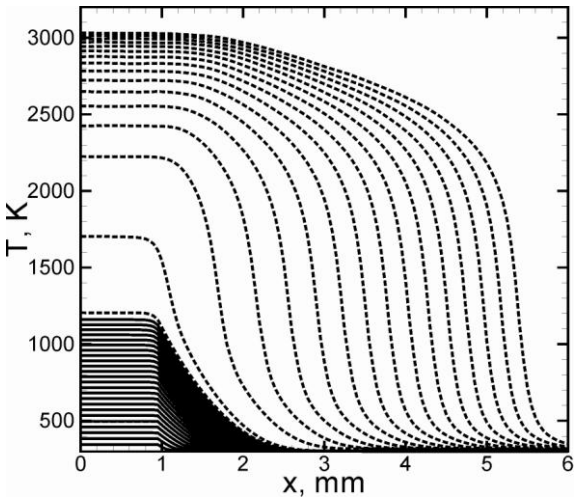
shown in Fig. 2 (b) demonstrates emerging of the spontaneous reaction wave and its coupling with the pressure wave leading to the detonation initiation through the Zeldovich mechanism. When Δt_Q is of the order of t_a and $t_a<\Delta t_Q$ the rarefaction wave has time to reach the center of the hot spot and to be reflected during the energy deposition. It may result in more complex non-uniformity formation however the mechanism of ignition remains the same.

For $\Delta t_Q < t_a < t_{ign}$ (for less amount of deposited energy) the gradient induced by the rarefaction wave forms on the stage after the end of energy addition. During the induction phase the acoustic perturbations equalize pressure in the hot spot and further ignition process evolves at the constant pressure out from the quasi steady temperature gradient. Combustion regime forming in this case depends on the environment conditions (e.g. pressure [2]): for example at $P_0 = 1atm$ such a temperature gradient causes deflagration wave, but at $P_0 = 10atm$ it causes detonation wave (similar to the case considered above for $L=1cm$ and $\Delta t_Q \sim 3\mu s$). In case of the rapid but relatively small energy deposition the resulting regime is a fast deflagration wave [2].

4 Millisecond Time Scale of Energy Deposition

If $t_a << \Delta t_Q \le t_{ign}$, then there is enough time for pressure to be equalized by acoustic waves and there are no strong compression waves emitted from the hot spot. The combustion regimes now depend essentially on the steepness of the temperature gradient, which is formed by the thermal wave and gas expansion in the vicinity of the hot spot. During Δt_Q the thermal wave propagates away from the hot spot at the distance $x_T / mm = (\chi \Delta t_Q)^{1/2} \approx 0.9(\Delta t_Q / ms)^{1/2}$. The expelled mass together with the thermal wave give rise to the temperature gradient in the surrounding mixture behind the boundary of the hot spot. The formed temperature profile is almost linear because of the weak temperature dependence of the coefficient of thermal conduction ($\kappa \propto T^{0.75}$). Fig. 3 shows the temperature gradient formed at the end of the energy deposition for $\Delta t_Q = 1000\mu s$, $L=1mm$ (solid lines). Such linear temperature gradient is too steep to initiate detonation through the Zeldovich gradient mechanism and the result is a deflagration wave. The thermal wave and the gas expansion are too slow to expand temperature and to form a temperature gradient compatible with the detonation formation at atmospheric or lower pressures [2]. Long before the thermal wave moves away on a sufficiently long distance the temperature of the mixture rises to ignite the reaction, so that either deflagration wave or fast deflagration wave are initiated [2]. In Fig. 3 dashed lines show the deflagration wave formation out from the formed temperature gradient.

Since coefficient of the thermal diffusivity does not depend on pressure one can create the same temperature gradient at higher pressures using the same millisecond scale energy source. The steepness of the temperature gradient for direct detonation initiation through the Zeldovich mechanism decreases considerably with the increase of pressure. Therefore the temperature gradient created by the thermal wave can trigger detonation at high enough initial pressure. This is shown in Fig. 4 for the hot spot $L = 1\text{mm}$ at initial pressure $P_0 = 10\text{atm}$. For a sufficiently long time of energy deposition the thermal wave creates the temperature gradient which initiates a detonation through the Zeldovich mechanism. Fig. 4 shows the temporal evolution of temperature and pressure profiles illustrating formation of the temperature gradient outside of the hot spot, the development of the spontaneous wave along the gradient and transition to detonation for $\Delta t_Q = 1\text{ms}$.



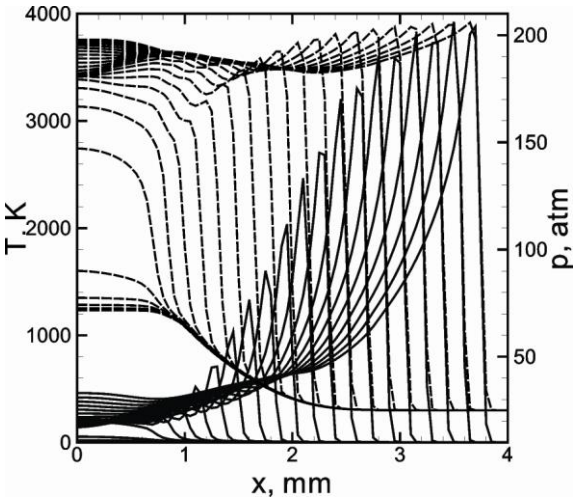


Figure 3 (left). Temperature profiles in the hot spot during (solid lines) and after energy deposition (dashed lines). $L = 1mm$, $P_0 = 1atm$ $\Delta t_Q = 1ms$. interval between profiles Δt=5μs.

Figure 4 (right). Evolution of temperature (dashed lines) and pressure (solid lines) profiles illustrating detonation formation on the gradient formed in the energy release region. $L = 1\text{mm}$, $\Delta t_Q = 1000\mu\text{s}$, $P_0 = 10\text{atm}$; interval between curves at the figure $\Delta t = 2\mu\text{s}$.

5 Ignition energy

The obtained results allow us to estimate the energy required for ignition of a particular combustion regime. At the same time it should be noted that the amount of the ignition energy obtained via extrapolating of the 1D calculations most likely will not match the actual value of the ignition energy for the 3D problem where the process is associated with a three-dimensional expansion and converging of the rarefaction wave. This difference is particularly important for the initiation of detonation. The three dimensional expansion additionally enhances the rarefaction. At the same time the shocks are weakened in course of the spherical expansion [4]. Both factors result in sufficient drop in temperature and pressure in the hot spot on the time scales of the order of acoustic time and lead to less suitable conditions for a detonation initiation. Thus, for the same conditions as in one-dimensional case the less intensive combustion regime arises. The deflagration regimes are less sensitive but to obtain detonation one should sufficiently increase the power of the energy source.

A large number of 3D simulations were used to verify realization of different combustion regimes and to compare the ignition energy obtained from 3D model compared to that extrapolated using the 1D model. As larger is the acoustic time t_a compared to the time of energy deposition as less the influence of the rarefaction wave on the detonation initiation. This means, that with the increase of the hot spot size ($t_a \sim L$) the initiation of detonation requires less power of the energy deposition into the specific volume of the hot spot for a given time of energy deposition, though the total deposited energy occurs to be larger compare to the case of detonation initiation in a smaller hot spot using higher power of the energy deposition. In particular, it is obvious that with the increase of the hot spot size, and corresponding increase of the acoustic time t_a, the role of rarefaction wave becomes less important.

6 Conclusions

In the present paper we used detailed chemical kinetics and transport models to study features of the localized transient energy deposition leading to the ignition of different regimes of combustion using as an example the stoichiometric hydrogen-oxygen mixture. It is shown that depending on the parameters of energy deposition (deposited energy amount, deposition time scale and size of the hot

spot) there are two main mechanisms of reaction wave initiation: the Zeldovich gradient mechanism [1] and the volumetrical thermal explosion (which actually represents one of the asymptotics of the Zeldovich mechanism for the gradient of zero steepness). For practically important time scales the principal scenarios of ignition are: 1) for sub-microsecond pulses the volumetrical explosion takes place inside the hot spot; 2) for microsecond-scale pulses the gradient of temperature and pressure arises on the profile created by the rarefaction wave and ignition starts via Zeldovich mechanism on the gradient of induction time; 3) for millisecond-scale pulses gasdynamical expansion gives rise for a temperature gradient at approximately constant pressure, and the ignition starts according to the Zeldovich mechanism [1] with all the features inherent to chain-branching chemistry disclosed in [2]. In three-dimensional case the spherical expansion of the hot spot weakens shock wave in favor of the intensified rarefaction wave. It results in sufficient drop in temperature and pressure in the hot spot on the time scales of the order of acoustic time. Thus, for the same conditions as in one-dimensional case the less intensive combustion regime arises.

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