Influence of Chemical Kinetics on Detonation Initiation by Temperature Gradients in H_2/air and CH_4/air Explosions

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ABSTRACT

Understanding the mechanisms of explosions is essential for the development of safety measured and for minimizing devastating hazards. Due to the complexity of real chemistry, a one-step reaction model has been often used for theoretical and numerical studies. In this paper we compare conditions for the detonation development from the spontaneous wave in a hot spot for a one-step model with that obtained for detailed chemical models. It is shown that for detailed chemical models conditions required for the detonation development from the spontaneous wave in a hot spot are more limited than that for the use of simplified chemical models. In particular, the minimum hot spot size capable of producing a detonation calculated with the detailed chemical model is at least an order of magnitude larger than that predicted by a one-step model even at high initial pressures. The impact of a detailed chemical model is particularly pronounced for the methane/air mixture, where not only is the hot spot size much greater than that predicted by a one-step model, but the initiation of detonation by the hot spot with a temperature gradient is possible only if the ambient temperature outside the gradient is above 1100 K.

KEYWORDS: detailed chemistry, spontaneous wave, detonation, explosion.

INTRODUCTION

Understanding the causes and mechanisms of explosions is essential for the development of safety measured and for minimizing devastating hazards in many industrial processes, such as coal mines, natural gas pipelines, hydrogen energy, nuclear, chemical and other industries [1-3]. Much experimental, theoretical and numerical work has been undertaken in an attempt to identify mechanism of the flame acceleration and the deflagration-to-detonation transition (DDT) [1, 4, 5]. Until recently a common approach to study DDT has been to use simulations based on a one-step chemical model [4, 5, 6] because complexity of real chemical kinetics. It was argued that the accelerating flame creates conditions in nearby unreacted material that ignite involving the Zel'dovich gradient mechanism and spontaneous reaction wave, and this is the mechanism of DDT. However, it was shown experimentally [7, 8] that for hydrogen/oxygen and ethylene-air mixtures the temperature in the vicinity of the flame prior to DDT does not exceed 550 K, which is too low for spontaneous ignition. Experimental studies and numerical simulations of DDT [8, 9, 10, 11] based on detailed chemical models for H_2/O_2 and H_2/air have shown that the DDT mechanism is different from the gradient mechanism. In this paper we consider the conditions for which the hot spots where the spontaneous reaction wave can undergo a transition to detonation through the Zel'dovich gradient mechanism for a one-step and for detailed chemical models in highly reactive H_2/air and in slow reactive CH_4/air. This may probably help in future (if this is possible in principle)

to try to optimize simplified models (e.g. ignition delay time as a parameter) to make them more reliable for simulations DDT.

INDUCTION TIMES: ONE-STEP AND DETAILED CHEMICAL MODELS

For H_2/air we consider the one-step Arrhenius model used in [12] for 2D simulations of the hydrogen/air flame acceleration and DDT in channel with obstacles.

$$W = A\rho Y \exp\left(-E_a/RT\right),$$ (1)

where all the parameters, the pre-exponential factor $A = 6.86 \cdot 10^{12}$ cm^3/(g·s), the gas density and the unburned mass fraction, ρ and Y, the activation energy of the reaction, $E_a = 46.37\, RT_0$, $\gamma = 1.17$ is the ratio of specific heats, etc. are the same as in [12]. The detailed mechanism for hydrogen/air chemistry is the mechanism developed by Kéromnès et al. [13], which consists of 19 reactions and 9 species. This mechanism was extensively validated over a large number of experimental conditions, especially focused on high pressures and it shows an excellent agreement between the modeling and experimental measurements.
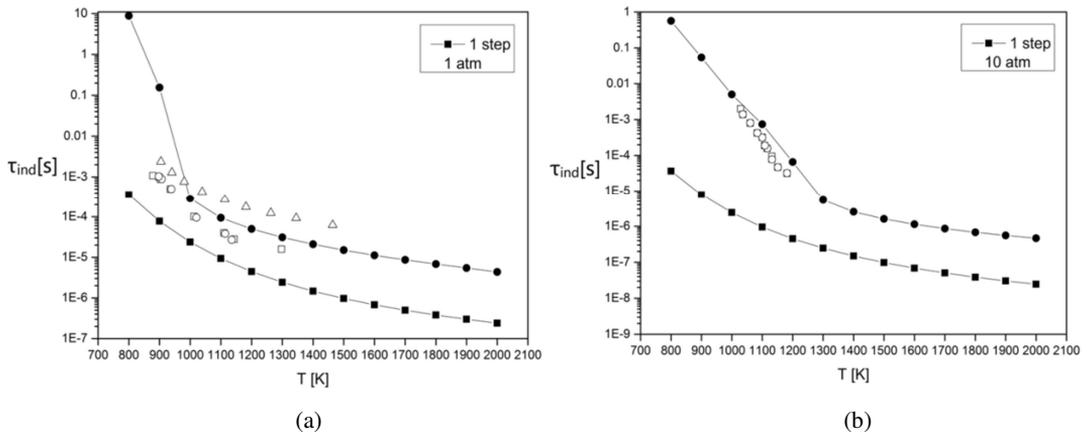

(a)   (b)

Fig. 1. Induction times for H_2/air calculated for the one-step and detailed models. (a) 1atm; (b) 10 atm. Empty symbols are experimental measurements. (a) □ − [15]; ○ − [16]; △ − [17]; (b) □ − [15], ○ − [18].

The one-step model for methane/air involves the same Eq.(1) used by Kessler et al. [6] for 2D simulations of the methane/air flame acceleration and DDT in a channel with obstacles. The same parameters as in [6] were used: $E_a = 67.55\, RT_0$, $A = 1.64 \cdot 10^{13}$ cm^3/(g·s), $\gamma = 1.197$, etc. The detailed model for CH_4/air is the detailed reaction mechanism DRM-19 developed by Kazakov and Frenklach [14], which consists of 19 species and 84 reactions. The DRM-19 mechanism was extensively validated by many researchers for combustion characteristics related to ignition delay times and laminar flame velocities over a wide range of pressures, temperatures, and equivalence ratios.

The ignition delay times were calculated for different chemical reaction schemes using the standard constant volume adiabatic model. The ignition delay time can be defined as the time during which the maximum rate of temperature rise, $\max\left(dT/dt\right)$, is achieved, which is close to the time of the exothermic reactions activation. Figures 1 (a, b) show the induction times for H_2/air versus temperature computed using the one-step model [12] and the detailed chemical model [13] at initial pressures $P_0 = 1$ atm and 10 atm. Open symbols indicate experimental measurements.

Figures 2 (a, b) show the induction times for methane/air at 1atm and 10atm computed for the one-step model [6], GRI 3.0 Mech, the detailed chemical model DRM-19 [14] and the experimental measurements (open symbols).

It is seen that the induction times predicted by the detailed chemical model are in a good agreement with the experimental results, but differ by up to three orders of magnitude from that predicted by the one-step model for H_2/air. Another feature of the "real" induction time is an abrupt change of $d\tau_{ind}/dT$ at the crossover temperatures, which correspond to the transition from the endothermal induction stage to the exothermal stage. The difference between the induction time given by the one-step model and the induction time calculated with the detailed chemical models for methane/air is about 10 times larger than it is for hydrogen/air.
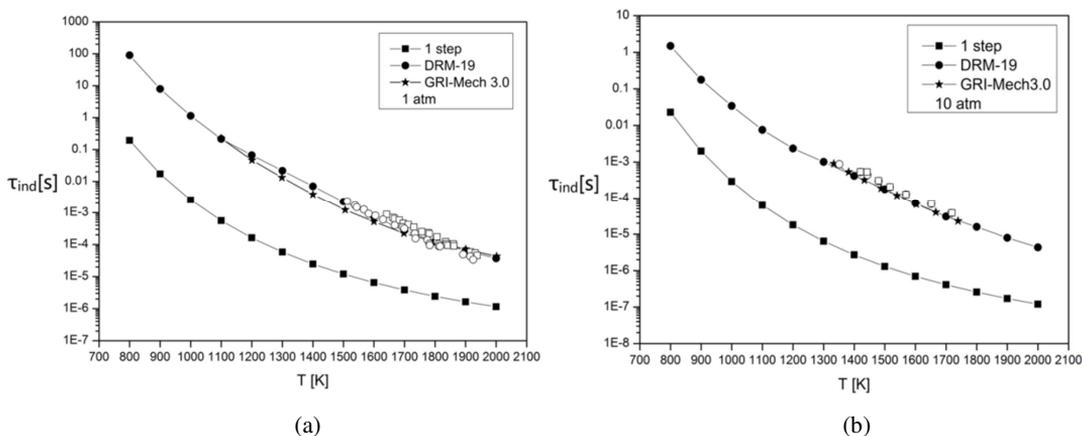

(a) (b)

Fig. 2. Induction times for CH_4/air calculated for the one-step and detailed models. (a) 1 atm; (b) 10 atm. Experiments: ○ – [19], □ – [20].

THE GRADIENT MECHANISM; SPONTANEOUS WAVES

We will use the conventional term a "hot spot", which is an area within a reactive mixture, where the temperature is higher than in the surrounding mixture. The scale of the temperature gradient in the hot spot $L = T / (dT / dx)$ is considered as the size of the hot spot.

The Zeldovich gradient mechanism

The ignition of a flammable mixtures is one of the most important and fundamental problems in combustion physics. In practical cases ignition begins in a small area of combustible mixture, which is locally heated by means of an electric spark, hot wire, and such like. Such local energy release results in the formation of an initially nonuniform distribution of temperature (or reactivity), which depending on the mixture reactivity and the initial pressure determines the evolution of the reaction wave. One needs to know how the initial conditions in such "hot spots" influence the regime of the reaction wave, which is ignited and propagates out from the ignition location. The question of how a hot spot can give rise to different combustion modes remained open until the Zel'dovich's concept [21] of the spontaneous reaction wave propagating along a spatial gradient of reactivity opened an avenue to study ignition of different regimes of the reaction wave that is initiated by the initial non-uniformity in temperature or reactivity caused by the local energy release [22]. In a region with nonuniform distribution of temperature the reaction begins at the point of minimum ignition delay time $\tau_{ind}(T(x)$ and, correspondingly, the maximum temperature, and then it spreads along the

temperature gradient by spontaneous autoignition at neighboring locations where τ_{ind} is longer. In the case of a one-step chemical model the induction time is defined by the time-scale of the maximum reaction rate. For a detailed chemistry this is the time scale of the stage when endothermic chain initiation completed and branching reactions begin. In the case of a one dimensional problem the spontaneous autoignition wave propagates relative to the unburned mixture in the direction of temperature gradient with the velocity:

$$U_{sp} = \left| \left(d\tau_{ind} / dx \right)^{-1} \right| = \left| \left(\partial\tau_{ind} / \partial T \right)^{-1} \left(\partial T / \partial x \right)^{-1} \right|, \tag{1}$$

Since there is no causal link between successive autoignitions, there is no restriction on the value of U_{sp}, which depends only on the steepness of temperature gradient and $\partial\tau_{ind} / \partial T$. It is obvious, that a very steep gradient (hot wall) ignites a flame, while a zero gradient corresponds to thermal explosion, which occurs within the induction time. The velocity of the spontaneous wave initiated by the temperature gradient decreases while the autoignition wave propagates along the gradient, and reaches the minimum value at the point close to the cross-over temperature [23], where it can be caught-up and coupled with the pressure wave, which was generated behind the high-speed spontaneous wave front due to the chemical energy release. As a result, the pressure peak is formed at the reaction front, which grows at the expense of energy released in the reaction. After the intersection of the spontaneous wave front and the pressure wave, the spontaneous wave transforms into a combustion wave and the pressure wave steepens into the shock wave. After the pressure peak becomes large enough, it steepens into a shock wave, forming an overdriven detonation wave. Classification of combustion regimes initiated by a temperature gradient has been studied in [21] for a one-step model, and for detailed chemical kinetics of hydrogen-oxygen and hydrogen-air in [23].

SPONTANEOUS WAVES AND TRIGGERING DETONATIONS

Problem setup

We consider uniform initial conditions apart from a linear temperature gradient within a hot spot. The model of the linear temperature gradient is convenient for analysis and it has been widely used in many previous studies. The initial conditions at $t = 0$, prior to ignition are constant pressure and zero velocity of the unburned mixture. At the left boundary $x = 0$ the conditions are for a solid reflecting wall, where $u(x,0) = 0$ and the initial temperature, $T = T^*$ exceeds the ignition threshold value. Thus, the initial conditions are quiescent and uniform, except for a linear gradient in temperature (and hence density):

$$T(x,0) = T^* - (T^* - T_0)(x / L), \ 0 \leq x \leq L, \tag{2}$$

$$P(x,0) = P_0, \ u(x,0) = 0 \tag{3}$$

The temperature gradient is characterized by the temperature $T(0,0) = T^*$ at $x = 0$, by the mixture temperature outside the hot spot, $T(x \geq L, 0) = T_0$ and by the gradient steepness, $(T^* - T_0) / L$. The "length" L, which characterizes the gradient steepness can be viewed as the size of the hot spot, at which the initial temperature gradient was formed.

The 1D direct numerical simulations are performed to solve the set of the one-dimensional time-dependent, fully compressible reactive Navier-Stokes equations and chemical kinetics. The equations of state for the reactive mixture and for the combustion products were taken with the temperature dependence of the specific heats and enthalpies of each species borrowed from the JANAF tables (Joint Army Navy NASA Air Force Thermochemical Tables) and interpolated by the

fifth-order polynomials. In the case of a one-step model the ideal gas equation of state was used. The viscosity and thermal conductivity coefficients of the mixture were calculated from the gas kinetic theory using the Lennard-Jones potential. Coefficients of the heat conduction of i-th species $\kappa_i = \mu_i c_{pi} / Pr$ are expressed via the viscosity μ_i and the Prandtl number, $Pr = 0.75$. Simulations of the time evolution of spontaneous wave and the detonation initiation were performed using fifth order conservative finite difference scheme (WENO). Thorough resolution (up to 5 µm) and convergence tests were performed to ensure that the resolution is adequate to capture details of the problem and to avoid computational artifacts. Because of limited space, we refer readers to Refs. [24, 25] for fuller details of the hydrodynamic solver and resolution tests.

Detonation initiation by temperature gradient in H$_2$/air

Figures 3(a, b) show the time evolution of a spontaneous wave and the detonation initiation by the steepest temperature gradient in H$_2$/air (the minimum hot spot size) at the initial $P_0 = 1$ atm computed for a one-step (3a) detailed (3b) models.
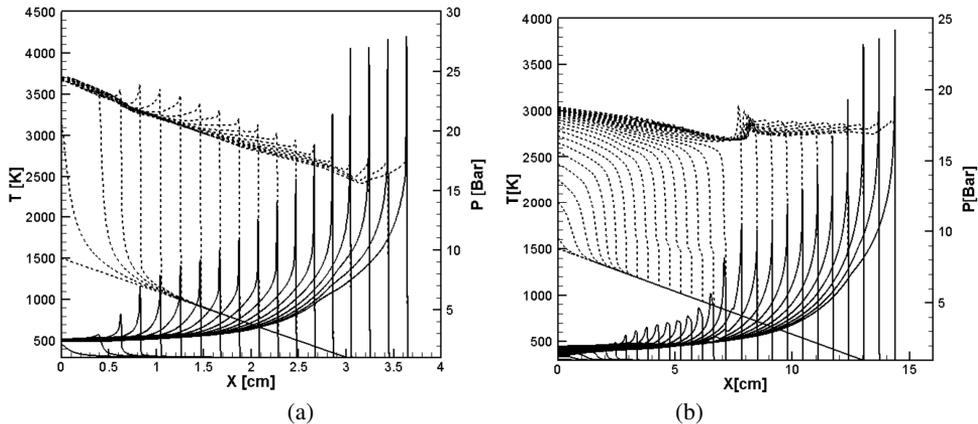

(a)   (b)

Fig. 3. Time evolution of the temperature (dashed lines) and pressure (solid lines) profiles during detonation initiation in H$_2$/air, at $P_0 = 1$ atm. (a) one-step model [11]; (b) detailed model [13].

The velocity at which the spontaneous reaction wave decreases, starts below the upper point of the gradient. If the gradient is sufficiently shallow, such that the minimum speed of the spontaneous wave is close to the sound speed $a_s(T_{cr}^*)$ at this point, the spontaneous reaction wave can couple with the pressure pulse produced by the energy released in the reaction. As a result, a pressure peak will grow at the expense of the energy released in the reaction. After the pressure peak has become large enough, it steepens into a shock wave, forming an overdriven detonation wave. For a steeper temperature gradient (larger size of the hot spot) the velocity of the spontaneous wave at the minimum point is not sufficient to sustain synchronous feedback amplification between the reaction and the pressure pulse. In this case, the pressure waves run ahead of the reaction wave, out of the gradient, and the result will be a deflagration, or fast deflagration, with weak shocks running away ahead of the flame.

The velocity of the spontaneous wave reaches its minimum value at the point close to the crossover temperature T_{cr}^*, which corresponds to the transition from the endothermal induction to the exothermal stage. Therefore, the necessary condition for initiating detonation by the spontaneous reaction wave is that the spontaneous wave initiated by the initial temperature gradient can be caught up and coupled with the pressure wave generated behind the high-speed spontaneous wave:

$$U_{sp}\left(T_{cr}^{*}\right)=\left(\frac{\partial \tau}{\partial T}\left(T_{cr}^{*}\right)\right)^{-1}\left(\frac{\partial T}{\partial x}\left(T_{cr}^{*}\right)\right)^{-1}=\left(\frac{\partial \tau}{\partial T}\left(T_{cr}^{*}\right)\right)^{-1}\frac{L}{T^{*}-T_{0}}\geq a_{s}\left(T_{cr}^{*}\right),\tag{4}$$

where T_{cr}^{*} at the point corresponding to $\min\{U_{sp}\}$ is slightly above the crossover temperature T_{cr}. Using this condition we can estimate the minimum size of the hot spot for the successful triggering detonation. Figures 4 (a, b) show velocities of spontaneous wave at the point $\min\{U_{sp}\}$ as a function of the hot spot size L calculated for the one-step (Fig. 4 a) and detailed (Fig. 4 b) models at P_0 = 1, 5, and 10 atm. At high pressures, when triple collisions dominate, the crossover temperature corresponding to the equilibrium of the induction and termination stages shifts to higher temperatures. Therefore, the minimum steepness of gradients for detonation initiation increases, but the corresponding minimum size of the hot spot ($L=L_{cr}$) required for triggering the detonation predicted by the one-step model remains much smaller than that predicted by detailed model.
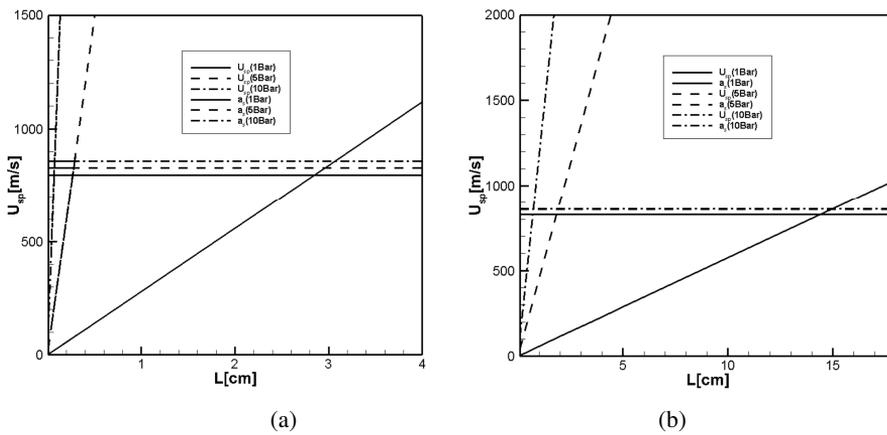

(a)   (b)

Fig. 4. $L=L_{cr}$ for H_2/air at P_0 = 1, 5, 10atm. (a): detailed model, T_{cr}^{*}(1 atm) = 1300 K, T_{cr}^{*}(5 atm) = 1400 K, T_{cr}^{*}(10 atm) = 1410 K. (b): one-step model T_{cr}^{*}(1 atm) = 1200 K, T_{cr}^{*}(5 atm) = 1300 K, T_{cr}^{*}(10 atm) = 1400 K.

(a)   (b)
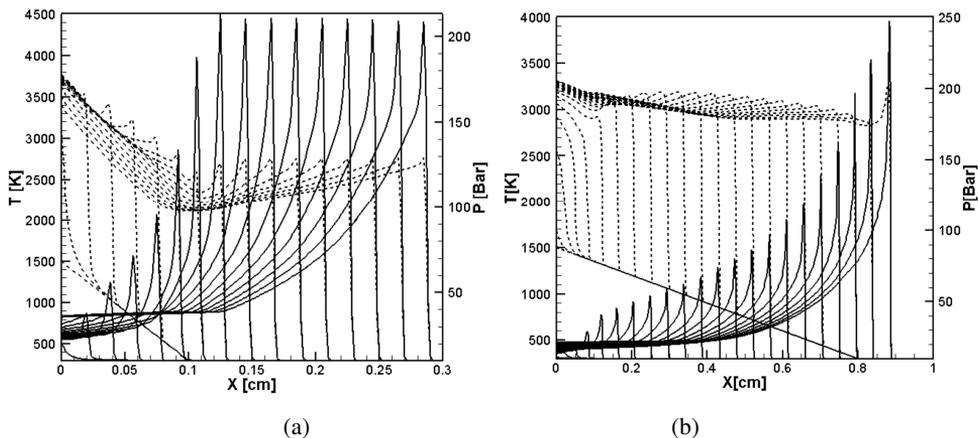
Fig. 5. Time evolution of the temperature (dashed lines) and pressure (solid lines) profiles during detonation initiation in H_2/air at P_0 = 10 atm. (a) one-step model; (b) detailed model.

Figures 5 (a, b) show the time evolution of temperature and pressure profiles during the initiation of detonation in H_2/air computed for one-step and detailed models at initial pressures 10 atm.

The hot spot sizes L_{cr}, at which the temperature gradient can produce a steady detonation for the one-step and for detailed models differ because of large difference in $\partial \tau_{ind}/\partial T$ for these models, which determines the speed of the spontaneous wave. The ratio of critical sizes of for detailed and one-step models is defined by large difference in $\partial \tau_{ind}/\partial T$ for the models

$$L_{cr_{det}}/L_{cr_{1-step}} \approx \left(\partial \tau_{ind}/\partial T \right)_{det} / \left(\partial \tau_{ind}/\partial T \right)_{1-step}. \tag{5}$$

Detonation initiation by temperature gradient in CH4/air

The induction times for methane/air are much longer for all temperatures compared to the hydrogen/air mixture. Therefore, the spontaneous wave velocity in methane/air is smaller for the same temperature gradients. Since the values of sound speeds and the Chapman-Jouguet velocities for H_2/air and CH_4/air are fairly close, one can expect that the minimum size of the hot spot, which can produce detonation in CH_4/air, will be about ten times greater than it is for H_2/air. Fig. 6 (a) shows the minimum size of the hot spot, which can produce detonation for the one-step model, but simulations with the detailed chemistry (Fig. 6 (b)) show that only a deflagration can be produced even for the hot spots, which was checked in simulations up to x > 50 cm..
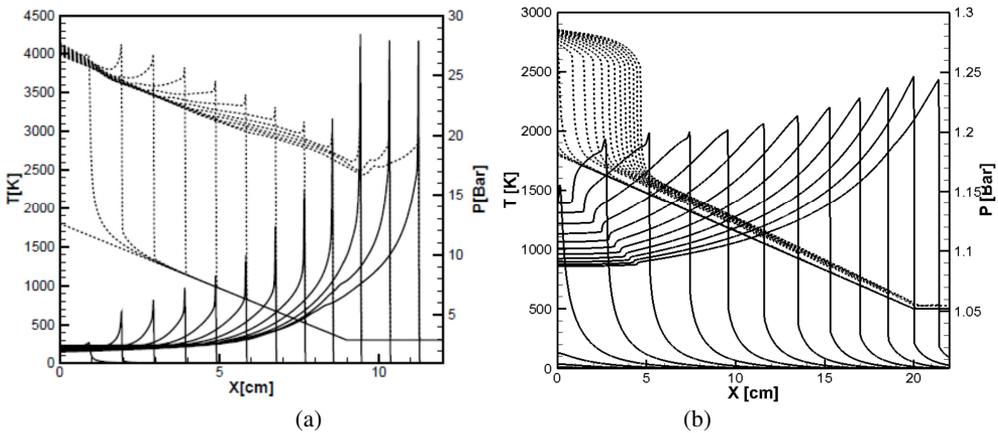

(a)   (b)

Fig. 6. Time evolution of the temperature (dashed lines) and pressure (solid lines) profiles for CH_4/air (P_0 = 1 atm, T_0 = 300 K, T^* = 1800 K). (a) one-step model [6]; (b) detailed model [14].

As the initial pressure increases, the induction time decreases, and the spontaneous wave speed increases rapidly. Therefore, at high pressures the minimum size of the hot spot capable of triggering detonation decreases. The minimum hot spot size, which can trigger detonation in CH_4/air at P_0 = 10 atm, T^* = 1800 K, T_0 =300 K, according to Eq. (4) could be L = 12 cm for the detailed DRM19 model. But in contrast to the scenario in Fig. 7 (a) calculated for the one-step model, the developing detonation in Fig.7 (b) quenches at x = 10 cm, even for a shallower temperature gradient, L = 20 cm. The reactive wave starts to move slowly away from the leading shock wave. The rarefaction wave propagates into the reaction zone and the separation between the heat release zone and the leading shock increases. As a result, the shock weakens and the detonation quenches. The phenomenon of spontaneous quenching of the developing detonation has been studied by He and Clavin [26, 27], who also pointed out that, for the same temperature gradient, for which a

detonation is quenching, a steady detonation can be ignited for a higher temperature T_0 outside the hot spot.

It was found that at the initial pressure 10 atm a steady detonation can be produced by the temperature gradient only if ambient temperature T_0 = 1100 K. Fig. 8 shows the evolution of temperature and pressure profiles during the development of a steady CJ-detonation from the temperature gradient L = 6 cm, T_0 = 1100 K. In a sense, high temperature outside the gradient is equivalent, but not completely, to a shallower gradient. The induction stage, which is distinctive for real chemical reactions can be "skipped" at sufficiently high ambient temperatures. The reaction front propagates at smoother ambient density, so that hydrodynamic resistance at the end and outside the gradient is smaller and the transition to detonation may occur for a steeper gradient [23].
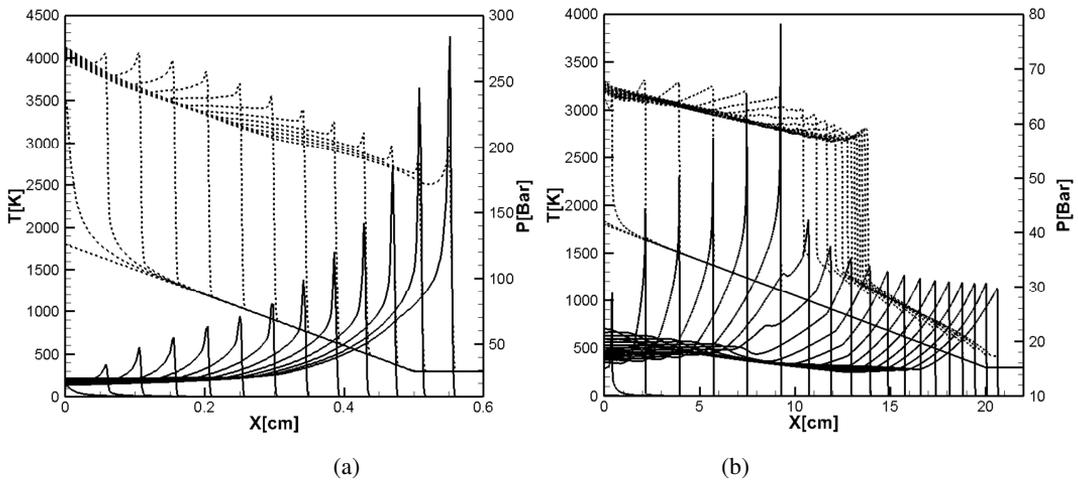

(a)   (b)

Fig. 7. Evolution of the temperature (dashed lines) and pressure (solid lines) profiles; P_0 = 10 atm, T_0 = 300 K, $T*$ = 1800 K. CH_4/air: (a) one-step model [6]; (b) detailed model [14].
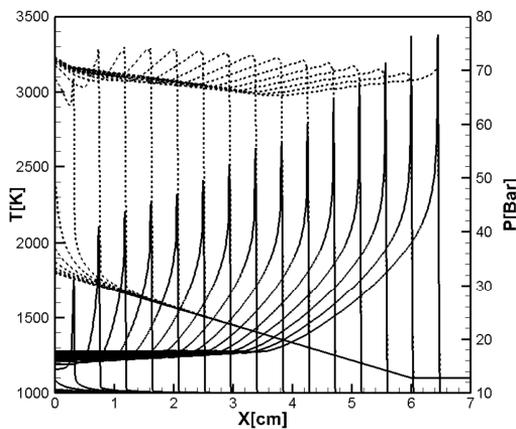

Fig. 8. Time evolution of the temperature (dashed lines) and pressure (solid lines) profiles during development of a steady detonation in CH_4/air for DRM19 model.

To verify the validity of the temperature of detonation, obtained in simulations we use the conservation laws. The value of reaction energy (q) obtained from conservation of energy for

deflagration: $C_{p2}T_b = C_{p1}T_1 + q$. Using this value of q and conservation of mass, momentum and energy, we obtain formulas for velocity and temperature of CJ detonation: $C_{v2}T_{CJ} = u_{CJ}^2 / \gamma_2(\gamma_2 - 1)$,

$$u_{CJ} = \left\{ \frac{\gamma_2 - 1}{2}\left((\gamma_2 + 1)q + (\gamma_1 + \gamma_2)C_{v1}T_1\right) \right\}^{1/2} + \frac{\gamma_2 - 1}{\gamma_2 + 1}\left\{ \frac{\gamma_2 + 1}{2}\left((\gamma_2 - 1)q + (\gamma_1 - \gamma_2)C_{v1}T_1\right) \right\}^{1/2}.$$

It should be noted that the temperature of detonation for a one-step model in Figs. 6 (a) and 7 (a), $T_{CJ} \approx 2820$ K is slightly above $T_{CJ} \approx 2700$ K for H$_2$/air. Since a steady detonation can be triggered by the temperature gradient only at high ambient temperatures ($T_0 = 1100$ K), the temperature of detonation shown in Fig. 8 calculated for detailed chemical model is $T_{CJ} \approx 3300$ K, in agreement with theoretical formulas for T_{CJ}.

CONCLUSIONS

The purpose of this study is to look more deeply into the influence of chemistry on the detonation initiation by a spontaneous wave developed by a temperature gradient for the highly reactive and low reactive mixtures. Although significant insights have been obtained through many experimental, theoretical and numerical studies, an identification of the basic mechanisms controlling deflagration-to-detonation transition remains one of the major challenges of combustion physics. Since interpretation of the multidimensional simulations, which used a one-step model, suggested that in most of the cases a spontaneous wave produced by the temperature gradient initiates detonation, it is important to know the real conditions when it is possible, and can be viewed as the mechanism of DDT. The results of high resolution simulations performed for one-step models were compared with simulations for detailed chemical models. The calculated values of induction times for H$_2$/air and for CH$_4$/air were validated against experimental measurements for a wide range of temperatures and pressures. It was found that the requirements, in terms of temperature and size of the hot spots, which produce a spontaneous wave, which in turn can initiate the detonation, are quantitatively and qualitatively different for one-step models compared to the detailed chemical models. The induction time and its temperature derivative of the induction time, which determines the speed of the spontaneous wave, are by orders of magnitude smaller for the one-step models, in comparison with the real values calculated for the detailed models and measured in experiments. As a consequence, for the one-step models the hot spots are much smaller and the temperature gradients initiating a detonation are much steeper than those calculated using detailed chemical models. The difference between the one-step and the detailed chemical model is more pronounced for low reactive CH4/air mixture. In this case, even at a high pressure of 10 atm, the minimum size of the hot spot, for which the spontaneous wave can initiate detonation, exceeds 6 cm and a steady detonation can be produced only for high ambient temperatures outside the hot spot exceeding 1100 K. Such a temperature can trigger a thermal explosion and is unlikely to be achieved during the flame acceleration prior to DDT. One of the conclusions is that the gradient mechanism of DDT, which was previously proposed on the basis of two-dimensional simulations using a one-step model, is unlikely at least in the case of methane/air. The results presented here may be used to improve the calibration of the simplified chemical-diffusive approach developed by Kaplan et al. [28], see also [6]. However, according to Fomin et al. [29] it seems to be impossible to calibrate simplified models so that they give a correct ignition delay times and even, more or less, correct burning velocities. The authors [29] used a 2-step model calibrated to reproduce induction times according to that measured in experiments, and they obtained excellent results for the cellular structure of detonation. But such a calibrated model does not describe correctly deflagration. For modelling DDT an accurate modelling of burning velocities and ignition delay times are required to predict correct run-up distances and mechanism of DDT. Therefore, an accurate modelling of burning velocities and ignition delay times are an absolute requirement.

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