



Influence of chemical kinetics on detonation initiating by temperature gradients in methane/air



Cheng Wang^a, Chengeng Qian^a, JianNan Liu^{a,b}, Mikhail A. Liberman^{c,*}

^a State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China

^b College of Mining Engineering, Taiyuan University of Technology, Taiyuan 030024, China

^c Nordic Institute for Theoretical Physics (NORDITA) Stockholm University, Roslagstullsbacken 23, Stockholm 10691, Sweden

ARTICLE INFO

Article history:

Received 30 May 2018

Revised 16 July 2018

Accepted 23 August 2018

Keywords:

Temperature gradient

Chemical models

Deflagration

Detonation

Explosions

Ignition

ABSTRACT

Different simplified and detailed chemical models and their impact on simulations of combustion regimes initiating by the initial temperature gradient in methane/air mixtures are studied. The limits of the regimes of reaction wave propagation depend upon the spontaneous wave speed and the characteristic velocities of the problem. The present study mainly focus to identify conditions required for the development a detonation and to compare the difference between simplified chemical models and detailed chemistry. It is shown that a widely used simplified chemical schemes, such as one-step, two-step and other simplified models, do not reproduce correctly the ignition process in methane/air mixtures. The ignition delay times calculated using simplified models are in orders of magnitude shorter than the ignition delay times calculated using detailed chemical models and measured experimentally. This results in considerably different times when the exothermic reaction affects significantly the ignition, evolution, and coupling of the spontaneous reaction wave and pressure waves. We show that the temperature gradient capable to trigger detonation calculated using detailed chemical models is much shallower (the size of the hot spot is much larger) than that, predicted by simulations with simplified chemical models. These findings suggest that the scenario leading to the deflagration to detonation transition (DDT) may depend greatly on the chemical model used in simulations and that the Zel'dovich gradient mechanism is not necessary a universal mechanism triggering DDT. The obtained results indicate that the conclusions derived from the simulations of DDT with simplified chemical models should be viewed with great caution.

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1. Introduction

Explosions of natural gas-air mixtures frequently occur in coal mines and natural gas pipelines and many other industrial processes. Understanding the causes and mechanisms of such explosions is essential for improving safety measures and minimizing devastating hazards. In the worst case explosions may be accompanied by the transition to detonation resulting in a considerable pressure rise and serious damage. Flame acceleration and possible mechanisms of the deflagration-to-detonation transition (DDT) leading to explosions have been extensively studied experimentally, theoretically and numerically [1–3].

If ignited in a confined area the flame accelerates and may undergo deflagration-to-detonation transition (DDT), which can present significant safety hazards. The fundamental mechanisms and processes by which a local small energy release in the reactive

mixture can lead to ignition of different chemical reaction modes is one of the most important and fundamental problems in combustion physics. One needs to know how combustion starts and how the transient energy deposition influences the regime of the reaction wave which propagates out from a finite volume of reactive gas where a transient thermal energy was deposited (the hot spot) [4]. This is important for improving safety measures and for understanding ignition risk assessments of processes where hydrocarbons are oxidized at different initial conditions of concentration, temperature and pressure.

A detonation can be initiated directly e.g., by strong shock waves via a localized explosion where a large amount of energy was released. An interesting possibility of the detonation initiation in hydrogen-air caused by focusing of shock waves reflected inside a wedge was recently studied by Smirnov et al [5]. However, in practical cases explosions almost universally start with the ignition of small flame in a relatively small area of combustible mixture where the ignition was initiated either by an electrical spark or another weak ignition source.

* Corresponding author.

E-mail addresses: michael.liberman@nordita.org, misha.liberman@gmail.com, mliber@nordita.org (M.A. Liberman).

A flame ignited near the closed end of a tube, accelerates and produces pressure waves which steepen into shocks in the flow ahead of the flame front. Various scenarios including shock waves, reflection of shock waves, viscous heating in the boundary layer can lead to the formation of hot spots with an inhomogeneous temperature or reactivity.

Methane-air explosions, and the transition to detonation in such explosions is an intricate problem. Due to the complexity of chemical kinetics for methane/air, until recently a common approach to study DDT has been simulations with a one-step Arrhenius chemistry model. A one-step model of chemical reaction is widely used for numerical simulations of flame dynamics for different geometry of channels (wide or thin) and for obstacle-laden channels in order to understand the mechanism of transition to detonation. The conclusion derived from these simulations was that the accelerating flame lead to the formation of hot spots, which can produce a detonation through the Zel'dovich gradient mechanism (e.g., [2,3,6–8]). To justify this approach Kessler et al. [8] argued that: “for many practical situations, an extensive description of the details of the chemical pathways is unnecessary. Instead, it is more important to have an accurate model of the fluid dynamics coupled to a model for the chemical-energy release that puts the released energy in the “right” place in the flow at the “right” time”. However, since the ignition times for a one-step model is by orders of magnitude shorter than the experimentally measured and calculated from detailed chemical models ignition times, the fluid dynamics model inevitably puts the released energy in the wrong place at the wrong time, no matter how accurate is the fluid dynamics model. It should also be noted that the flame velocity-pressure dependence given by a one-step model also does not agree with the experimentally measured velocity-pressure dependence. Therefore, results of the simulations of DDT with simplified chemical models should be considered with great caution.

For the first time possible regimes of propagating chemical reaction wave ignited by the initial temperature gradient were studied by Zel'dovich et al. [9] using a one-step Arrhenius model. The Zel'dovich's concept [10] of the spontaneous reaction wave propagating through a reactive mixture along a spatial gradient of reactivity is of great fundamental and practical importance. It opens an avenue to study the reaction ignition and different regimes of the reaction wave propagation initiated by the initial non-uniformity in temperature or reactivity caused by the local energy release.

In a region with nonuniform distribution of temperature the reaction begins at the point of minimum ignition delay time (induction 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 the realistic case of a chain branching chemistry this is the time scale of the stage when endothermic chain initiation completed and branching reactions begin. In the case of a one dimension gradient of temperature the spontaneous autoignition wave propagates relative to the unburned mixture in the direction of temperature gradient with the velocity, which is inversely proportional to the gradient of the induction time:

$$U_{sp} = |(d\tau_{ind}/dx)|^{-1} = |(\partial\tau_{ind}/\partial T)^{-1}(\partial T/\partial x)^{-1}|. \quad (1)$$

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. It is obvious, that a very steep gradient (hot wall) ignites a flame, while a zero gradient corresponds to uniform explosion, which occurs in the induction time. For a finite value of the temperature gradient Zel'dovich and co-workers have shown that a sufficiently shallow initial

temperature gradient can ignite a detonation regime of combustion [9]. The velocity of 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 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 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.

Obviously, a simplified one-step and even more advanced two-step or four-step models, which to some extent mimic the chain-branching kinetics, do not describe properly systems governed by a large set of chain-branching reactions. The quantitative and in some cases qualitative difference between simplified models and detailed chemical models remained unclear. Liberman et al. [11,12] employed detailed chemical kinetic schemes to study the combustion regimes in stoichiometric hydrogen-oxygen and hydrogen-air mixtures ignited by the initial temperature gradient. It was shown that the evolution of a spontaneous wave calculated using the detailed kinetic model is qualitatively different compared with the predictions obtained from calculations with a one-step model. First, the induction times predicted by a one-step Arrhenius model are in orders of magnitude smaller than the induction times predicted by a detailed chemical model. Another difference is that for the one-step model the reaction is exothermic for all temperatures, while chain branching reactions start with endothermic induction stage representing chain initiation and branching. Therefore, for a detailed model the hydrodynamics is effectively “switched-off” during induction stage. As a consequence, combustion regimes initiated by the temperature gradient require much shallower gradients compared with those predicted by a one-step model. This means that the size of a hot spot with a temperature gradient capable of producing detonation obtained in simulations with a detailed chemical model can be by orders of magnitude greater than that obtained from simulations with a one-step model. The size of a hot spot with a temperature gradient capable of producing detonation decreases with the increase of initial pressure [12], and may become rather small at very high pressure for hydrogen-air [13].

From the results of simulations with a one-step model, the Zel'dovich gradient mechanism is often considered as a universal mechanism explaining the transition from deflagration to detonation [2,3,6–8]. This trend was considered as the mainstream in DDT studies until it was shown experimentally by Kuznetsov et al. [14] that for a stoichiometric hydrogen/oxygen and ethylene-air mixtures the temperature in the vicinity of the flame prior to DDT remains too low (does not exceed 550 K) for spontaneous ignition. Experimental studies and numerical simulations of DDT with the detailed chemical model for hydrogen/oxygen [15–18] have shown that the gradient mechanism cannot explain DDT. A new mechanism of DDT consisting in the mutual amplification of a weak shock formed very close ahead of the flame front and coupled with the flame reaction zone was proposed by Liberman et al. [14]. This mechanism of DDT is basically very similar to the SWACER mechanism (shock wave amplification by coherent energy release) proposed by Lee and Moen [19], and the similarity of the SWACER mechanism and coherent amplification of the shock wave and the flame reaction is the probable reason that the results of simulation with a one-step chemical model were often interpreted as the spontaneous wave formation following by the onset of detonation via the gradient mechanism.

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