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Effects of thermal radiation heat transfer on flame acceleration and transition to detonation in particle-cloud hydrogen flames



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ABSTRACT

The current work examines regimes of the hydrogen-oxygen flame propagation and ignition of mixtures heated by radiation emitted from the flame. The gaseous phase is assumed to be transparent for the radiation, while the suspended particles of the dust cloud ahead of the flame absorb and reemit the radiation. The radiant heat absorbed by the particles is then lost by conduction to the surrounding unreacted gaseous phase so that the gas phase temperature lags that of the particles. The direct numerical simulations solve the full system of two phase gas dynamic time-dependent equations with a detailed chemical kinetics for a plane flames propagating through a dust cloud. It is shown that depending on the spatial distribution of the dispersed particles and on the value of radiation absorption length the consequence of the radiative preheating of the mixture ahead of the flame can be either the increase of the flame velocity for uniformly dispersed particles or ignition either new deflagration or detonation ahead of the original flame via the Zel'dovich gradient mechanism in the case of a lavered particle-gas cloud deposits. In the latter case the ignited combustion regime depends on the radiation absorption length and correspondingly on the steepness of the formed temperature gradient in the preignition zone that can be treated independently of the primary flame. The impact of radiation heat transfer in a particle-laden flame is of paramount importance for better risk assessment and represents a route for understanding of dust explosion origin.

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1. Introduction

Hydrogen has emerged as an important fuel in a number of diverse industries as a means of achieving energy independence and to reduce emissions. Nowadays, when hydrogen technologies and fuel cells are penetrating the market in a number of applications, extensive research is still needed for effectively addressing the high-risk technological barriers in a pre-competitive environment. Widespread deployment and use of hydrogen and hydrogenbased technologies can occur only if hydrogen safety issues have been addressed in order to ensure that hydrogen fuel presents at least the same level of hazards and associated risk as conventional fuel technologies. Hazard identification is the necessary step to ensure the full and safe utilization of hydrogen in either hydrogen safety engineering or risk assessment. The purpose of the hazard identification is to identify all events that can affect facility

* Corresponding author. E-mail address: mliber@nordita.org (M.A. Liberman). operation leading to a hazard to individuals or property. Since hydrogen is considered as extremely flammable and easily detonable gas when mixed with air over a wide range of composition, explosion hazards associated with the production, transportation and storage of hydrogen must be resolved to a sufficient confidence level and the key challenges facing the future widespread use of hydrogen are safety-related issues.

The hazardous potential of hydrogen—air and hydrogen—oxygen mixtures has been extensively studied and a huge number of experimental, theoretical and numerical studies inspired by their importance for industrial safety had been taken in attempt to understand nature of the explosion (Bentaib et al., 2015; Gupta, 2015; Mannan and Lees, 2005; Flame Acceleration, 2000; Kikukawa et al., 2009; Pasman, 2011; Eichert and Fischer, 1986; Ng and Lee, 2008; Eckhoff, 2009). Although most accidental explosions are deflagrations, in the worst-case scenario, the flame acceleration can lead to deflagration-to-detonation transition (DDT). Depending on the mixture characteristics, such as concentrations, temperature, pressure and flow geometry, combustion process can undergo strong flame acceleration and deflagration-to-detonation transition (DDT). These regimes are characterized by high burning rates and consequently by high pressure loads. The resulting detonation is extremely destructive, can induce pressures up to or above 10 MPa, and therefore can have especially catastrophic consequences in a variety of industrial and energy producing settings related to hydrogen. Since the discovery of detonation more than 150 years ago, a huge number of experimental, theoretical and numerical studies had been taken in attempt to understand nature of the transition from deflagration to detonation (see e.g. Ciccarelli and Dorofeev, 2008; Oran and Gamezo, 2007 and references within). These studies are inspired by their importance for industrial and nuclear power plants safety as well their potential application for micro-scale propulsion and power devices (Roy et al., 2004; Smirnov et al., 1999). Despite many years of substantial achievements in the area of the flame acceleration and DDT, still many specific aspects of the problem remain unclear. Dependence of the potential danger of the combustion process appeared to be very sensitive to the geometrical conditions of the processes, mostly to the confinement and to the congestion of the volume. Currently a unified physical model and corresponding numerical instrument which can be used over the entire range of phenomena is not available. Numerous combustion models are usually addressing only specific regime or phenomenon and are applicable only in their domain of validity.

The hazardous potential of hydrogen-oxygen and hydrogen-air mixtures has been extensively studied assuming a perfect mixture of hydrogen fuel and oxidant. Since the pioneering studies by Shchelkin, Zeldovich, Oppenheim and their co-authors (Shchelkin, 1940: Shchelkin and Troshin, 1965: Zel'dovich and Kompaneets. 1960; Urtiew and Oppenheim, 1966) there has been a continuous efforts aiming to elucidate a reliable physical mechanism explaining DDT. From the beginning there was widely spread opinion that turbulence plays a key role in the flame acceleration and DDT. A common belief was that a fast flame acceleration and the transition to detonation can occur only for strongly turbulent flames. Since the very first DDT studies it was known that the presence of obstacles increases the flame acceleration and shortens considerably the run-up distance. The experiments demonstrated that a flame accelerates more rapidly toward the open end of a duct if it passes through an array of turbulence-generating baffles. This presumably was the reason why the first attempts to explain DDT were associated with turbulent flames and were based on the assumption that DDT might occur only in the case of turbulent flames. Channels with rough walls or obstacles are often used to study DDT since it is believed that in this case the run-up distance is more or less fixed and controlled by turbulence (Teodorczyk et al., 2009; Wen et al., 2015). However, recent large scale experiments (Proust, 2015) with different kind of mixtures (C₂H₄-air, CH₄-air, C₃H₈-air, H₂-air) suggest that the self-acceleration mechanism of the flame may be much better represented by flame instabilities than by turbulence build-up. All the same DDT is easily observed in channels with smooth walls (Kuznetsov et al., 2005, 2010; Liberman et al., 2010) and in thin capillary tubes (Wu et al., 2007). The first explanation of the flame acceleration in tubes with no-slip walls before the DDT occurred was given by Zel'dovich (Zel'dovich, 1947). In his detailed analysis of the Shchelkin's experimental results Zel'dovich has pointed that turbulence is not a primary factor responsible for flame acceleration in a smooth-walled channel and sequential detonation formation. Explaining the nature of the flame acceleration in the DDT events Zel'dovich emphasized that the flame acceleration in a tube with no-slip walls is due to stretching of the flame front caused by the flame interaction with a nonuniform velocity field of the upstream flow, while turbulence plays a supplementary role if any depending on the experimental conditions. Although the qualitative picture of the DDT is more or less clear, however a quantitative theory and the physical mechanism of DDT are still poorly understood and require better theoretical and physical interpretation. With the advance in scientific computing, research has been shifted towards the use of computational approaches. Nowadays, numerical simulations can provide a qualitative picture of the basic processes from ignition and flame acceleration up to the transition to detonation. The reviews (Ciccarelli and Dorofeev, 2008: Oran and Gamezo, 2007) summarize the numerical efforts undertaken in the past decades to understand the deflagration-to-detonation mechanism in a highly reactive gaseous mixtures (e.g. hydrogen/air, acetylene/air) using a one-step Arrhenius chemical model. The conclusion drawn from these studies was that the mechanism of DDT is the Zeldovich gradient mechanism (Zel'dovich, 1980) involving gradient of reactivity. However, as an unsteady process, DDT involves multiple processes of vastly different scales. Among them, complex chemical reactions play a first-order controlling role for gaining scientific insight into the mechanism of DDT (Liberman, 2014). The numerical study of the Zeldovich gradient mechanism using a detailed chemical reaction models for hydrogen/oxygen and hydrogen/air (Liberman et al., 2011, 2012) has shown that the minimum scale of the temperature gradient (the length-scale of the temperature inhomogeneity) capable to initiate detonation exceeds size of the hot spots formed in the unreacted material ahead of accelerating flame by orders of magnitude. Recent 2D and 3D numerical simulations of the flame acceleration and DDT in hydrogen-oxygen mixtures that have taken into account a detailed chemical kinetics have revealed an adequate mechanism of DDT (Liberman et al., 2010; Ivanov et al., 2011a. 2011b. 2013: Machida et al., 2014).

An important problem of "hydrogen safety" is connected with leakage of the hydrogen and its further explosion. Hydrogen release might occur on storage, transport and handling. Once a flammable mixture forms, it can be ignited by a variety of uncontrolled means. An ignition is likely for all forms of releases due to the wide range of flammability and low ignition energy. The destructive power of the resulting explosion depends on the volume of the reactive mixture, its composition, and the geometries of confinement. In most practical cases ignition arises from a small area of combustible mixture, as an accidental ignition e.g. from an electric spark, or any local heating and starts as a laminar flame. The flame evolution can result in substantial flame acceleration, depending on the geometries of confinement, e.g. friction of the wall results in the flame front stretching, obstacles may result in flame turbulization, etc. Mechanisms of ignition by transient energy deposition and different scenarios of a detonation initiation were investigated in (Kiverin et al., 2013).

Most of studies on dust explosions have been performed to examine the characteristics or the indices of dust explosions in a closed vessel (Eckhoff, 2009). The fundamental mechanisms of flame propagation in dust suspension, however, have not been sufficiently studied and the limited experimental results known in the literature are often contradict each other. In particular, the influence of radiative heat transfer on the rate of flame propagation and duct cloud explosions is not yet fully understood. Combustion of the hydrogen-oxygen and hydrogen-air mixtures was studied largely at standard environmental conditions, however new technologies often dictate substantial variation of the conditions which have to be taken into account for the safety analysis. Among others, the fundamental properties of hydrogen mixtures with dusts of fine particles have to be considered. Non-uniformities of the gas distribution and small, micron-size solid particles suspended in the gas mixture can considerably affect regime of combustion in some cases leading to the strong flame acceleration and DDT. However, only limited amount of the experimental data are available on the behavior of the hydrogen in the presence of suspended particles Download English Version:

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