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Large-scale flame structures in ultra-lean hydrogen-air mixtures

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ARTICLE INFO

Article history:

Received 2 September 2017

Received in revised form

30 October 2017

Accepted 23 November 2017

Available online xxx

Keywords:

Ultra-lean hydrogen-air flames

Hydrogen safety

Numerical modeling

Flame balls convective transport

ABSTRACT

The paper discusses the peculiarities of flame propagation in the ultra-lean hydrogen-air mixture. Numerical analysis of the problem shows the possibility of the stable self-sustained flame ball existence in unconfined space on sufficiently large spatial scales. The structure of the flame ball is determined by the convection processes related to the hot products rising in the terrestrial gravity field. It is shown that the structure of the flame ball corresponds to the axisymmetric structures of the gaseous bubble in the liquid. In addition to the stable flame core, there are satellite burning kernels separated from the original flameball and developing inside the thermal wake behind the propagating flame ball. The effective area of burning expands with time due to flame ball and satellite kernels development. Both stable flame ball existence in the ultra-lean mixture and increase in the burning area indicate the possibility of transition to rapid deflagrative combustion as soon as the flame ball enters the region filled with hydrogen-air mixture of the richer composition. Such a scenario is intrinsic to the natural spatial distribution of hydrogen in the conditions of terrestrial gravity and therefore it is crucial to take it into account in elaborating risk assessments techniques and prevention measures.

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Introduction

For decades combustion processes in lean gaseous mixtures have been a subject of study for numerous research groups worldwide. Apart from fundamental problems of the combustion theory, topics related to the combustion of the fuel-lean mixtures arise due to a wide diversity of its applications for many branches of industry and energy sector. Low emission of nitric oxides and other greenhouse gases defines the prospects of the propulsion devices and power plants that utilize lean combustion processes [1]. Moreover, the detailed study of the lean flames features is of great concern when solving the issues related to fire and explosion safety [2]. In

particular, problems of assessment and minimization of potential risks of ignition of the combustible mixtures formed as a result of abnormal fuel emissions into surrounding atmosphere are of paramount interest [3]. Studying accidents, which develop according to this scenario, special attention should be paid to combustion of the hydrogen-air mixtures. Ejection of hydrogen into the surrounding air is possible in various emergency situations, including accidents at the nuclear power plants [4], where hydrogen is gradually accumulated in the atmosphere under containment as a result of the uncontrolled zircaloy oxidation process. At the same time, hydrogen is the perspective fuel, so the issues of its storage and transportation safety inevitably arise [5]. Depressurization of the hydrogen fuel tanks and pipelines is also one of the

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<https://doi.org/10.1016/j.ijhydene.2017.11.138>

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possibilities of the flammable mixture formation. In case of the hydrogen injection into the large confined spaces, formed combustible mixture composition could vary in a wide range. Herewith the hydrogen could be distributed non-uniformly in space [6], and locally the combustible mixture could have ultra-lean composition with equivalence ratio close to the lean flammability limit. Despite the low burning velocities and moderate pressure and thermal loads caused by such lean mixtures burn out, serious risks could be related with convective transfer of the lean flame into the location occupied with more chemically active composition (in case of natural vertical stratification of hydrogen [6]) and its subsequent ignition, so more hazardous combustion processes could develop, such as fast deflagration or even detonation [7]. All these considerations should be taken into account when formulating the risk mitigation measures and designing of the reliable explosion safety systems.

In the hydrogen-air mixtures of near-stoichiometric and lean composition (with hydrogen content larger than 10%) the combustion propagates in a classic deflagration regime, that is widely discussed in a number of papers [8,9]. As the lean flammability limit is approached, at hydrogen content less than 10%, the main physical mechanism of the flame propagation switches from thermal diffusion to deficient specie diffusion into the reaction zone. Ya. B. Zel'dovich first theoretically predicted the possibility of the purely diffusive spherical flames formation in the ultra-lean mixtures or the so-called flame balls [10]. He provided theoretical analysis which implies that these structures are intrinsically unstable. However further theoretical and experimental studies shown that external forces such as gravity [11,12] or heat losses due to radiation [13,14] or heat transfer to the cold walls [15] in microgravity conditions can stabilize ultra-lean flames.

Flame propagating in the ultra-lean mixtures with Lewis number lower than unity under terrestrial gravity conditions is subjected to various instabilities such as hydrodynamic instability (Darrieus-Landau instability), thermo-diffusive instability proposed by Zeldovich, Barenblatt and Sivashinsky and buoyancy-induced convective instability, which develops according to the general Rayleigh-Taylor mechanism. It is rather difficult to distinguish the influence caused by one or another instability on the flame propagation dynamics in the practically important environments that are characterized by complex geometries and terrestrial gravity force. One of the common ways to simplify the analysis is to conduct studies in microgravity or zero-gravity conditions, where the effects related with natural convection are negligible and the main role belongs to the thermo-diffusive instability development. A large number of theoretical and experimental studies in microgravity allowed to determine many significant features of the near limit lean flames. As it turned out, for mixtures with $Le < 1$ flame curvature intensifies combustion [14]. This feature of the lean flame is crucial for its stable propagation. Also, flammability limits and flame propagation regimes under the influence of thermo-diffusive instability were thoroughly examined at microgravity conditions. However, these results are not sufficient for solving practical fire and explosion safety issues at terrestrial gravity conditions. Convective transport of the flame and gas-dynamical flows induced by the flame motion should be taken into account as

they can alter flammability limits, flame propagation velocities and affect the observed flame structure. Theoretical studies have shown that convection-induced instabilities have a crucial impact on the slow ultra lean flames and stabilize flame structure during flame upward propagation [16,17]. Further numerical simulations proved theoretical estimations [12,18] for lean H_2 - O_2 - N_2 mixtures and reproduced initial stages of the flame propagation out from the ignition source and formation of the cap-shaped flame structures observed in experiments [19,20].

It is useful to note that ultra-lean flame is subjected to the gas-dynamical factors related with expansion of hot combustion products in different manner than widely studied freely propagating deflagrative flames [21,22]. First of all, lower reactivity of the ultra-lean compound does not provide sufficient rate of heat release for stable deflagration wave formation. Due to this fact expansion factor is not enough for stable outwardly flame propagation. In case of microgravity a stable flame ball is formed supported by the diffusion mechanisms discussed above. In case of terrestrial conditions the main upward direction of flame propagation establishes due to buoyancy of hot products. In addition to this the low value of burning rate does not provide intensive rise of intrinsic Landau-Darrieus instability [21,23] at the background of outward flame propagation in the terrestrial gravity field.

However, discussed studies were mainly aimed on fundamental analysis of various features of ultra-lean flames and were abstracted from the issues related to fire or explosion safety. In particular, a detailed analysis of the combustion dynamics and its stability mechanisms in the real-scale domain is necessary to prevent accidents caused by the convective transfer of the flame in the lean mixture. A significant effort in this direction was made in Refs. [24–26], where H_2 - CH_4 -air lean flames were stabilized in the cylindrical burner and analyzed both experimentally and numerically. Important results on ultra-lean flame structure, its stability, and issues related to its numerical modeling were obtained by the authors. However, dynamics of freely propagating ultra-lean flames affected by natural convection in large-scale domains is still not thoroughly examined. In this study, we present novel results on numerical simulation of the non-stationary flame propagation in the large-scale domain filled with the ultra-lean hydrogen-air mixture that can be used for solving real issues in a field of hydrogen safety.

Problem setup and numerical method

In this paper, we solved numerically the problem of flame ball formation and propagation in the semi-unconfined space filled with the ultra-lean hydrogen-air mixture with 6% hydrogen content at normal initial conditions ($T = 300$ K, $p = 1$ atm). Numerical domain represented half-space confined with the wall from the bottom and outlet conditions on the top and both sides. Bottom wall temperature was equal to the ambient temperature of the mixture ($T_{wall} = 300$ K). The ignition of the mixture was modeled with the instantaneous energy input into the small region corresponded to the local mixture heating up to 1500 K. Schematically the problem setup is shown in Fig. 1. In addition, to understand the geometry effect on the stability of

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