Flame Propagation through Ultra-Lean Hydrogen-Air Mixture under Terrestrial Gravity Conditions

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ABSTRACT

The paper is devoted to the study of peculiarities of flame dynamics in ultra-lean hydrogen-air mixtures in terrestrial gravity conditions. By means of numerical methods, it is shown that gas-dynamical flows, which develop due to buoyancy force exerted on hot combustion products, play a crucial role on the overall ultra-lean flame dynamics from the earliest stage after ignition and up to large-scale motion of the developed flame. Immediately after ignition convective flows determine the flame kernel stability. It is shown that despite the superadiabatic temperature of the flame products that is considered as one of the main stability factors of the ultra-lean flames in microgravity conditions the influence of convective flows on the ultra-lean flames in terrestrial gravity conditions can alter flammability limits from that measured in microgravity. On the other hand, the propagation dynamics of the stable flame kernels is also mainly determined by the buoyancy forces. Rising velocity of the flame kernel in the ultra-lean mixture occurs to be much greater than burning velocity and correlates well with estimations obtained for the bubble rising in liquid. Apart from the upward rising, the developed flame is shown to be expanding laterally so the complex large-scale flame structure is observed which could be a possible hazard of explosion and fire for many industrial environments.

KEYWORDS: Ultra-lean flames, hydrogen safety, numerical modeling, flame ball.

INTRODUCTION

Abnormal leakage of flammable gases into the atmospheric air inside the confined chambers poses a serious threat of fire and explosion. The most dangerous conditions arise when the chamber volume is rather small so almost perfectly stirred stoichiometric composition of the combustible gas with the atmosphere is formed inside the chamber. In this case, accidental ignition can result in combustion wave propagating in such devastating regimes as fast deflagration or even detonation. However, in a real emergency situation stoichiometric composition of the combustible mixture is rarely observed. In case of low leakage rates of the flammable gas together with large room volume, formed combustible mixture could be of overall lean composition. Combustion of the lean mixtures, despite being less harmful compared to fast deflagration and detonation, can result in ignition of more chemically active substances or cause malfunction of equipment and have to be considered as a potential danger as well. Taking into account current developments aimed at deployment of hydrogen as a perspective environmentally friendly fuel and possible accidental scenarios on nuclear power plants involving hydrogen accumulation in the atmosphere under containment, it is of great importance to analyse details of flame propagation in lean hydrogen-air mixtures including ultra-lean compositions.

Lean combustion is a subject for extensive experimental and theoretical studies in the last decades. Usually, those studies were performed in microgravity conditions that allowed obtaining significant

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results on flammability limits and stabilization mechanisms of those flames [1]. However, features of the lean flames subjected to terrestrial gravity conditions are still poorly investigated and understood, despite it is of crucial importance for practical fire safety applications. The aim of the present paper is to analyse by means of numerical modelling lean hydrogen-air flame structure and stability under terrestrial gravity conditions.

PROBLEM SETUP

To understand features of flame dynamics in ultra-lean gaseous mixtures we consider the following problem setup (see Fig. 1). Semi-unconfined space is filled with the ultra-lean hydrogen-air mixture with 5-9 vol% hydrogen content (corresponding equivalence ratios $\varphi = 0.125$ -0.235) at normal initial conditions (T = 300 K, p = 1 atm). Hydrogen-air mixtures are considered firstly due to a large amount of accumulated data on hydrogen combustion and secondly due to perspectives of hydrogen use as a green fuel. The bottom wall is isothermal and its temperature is equal to the initial ambient temperature of the mixture ($T_{\text{wall}} = 300 \text{ K}$). The numerical ignition of the mixture occurs near the bottom wall in the small region instantly "heated up" to 1500 K. Terrestrial gravity force is taken into account, gravity acceleration value $g = 9.8 \text{ m/s}^2$. For reference cases from the hydrogen concentration range 5-6 vol% the cell size of the Cartesian numerical grid was taken equal to 0.2 mm, which is in convergence region for one-dimensional flame velocity tests carried out in advance. For the richer concentration region (8-9 vol%) a finer grid (0.1 mm) was used.

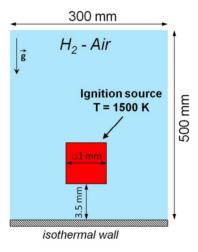


Fig. 1. Problem setup.

Governing equations represent a gas-dynamical model in the low-Mach number approximation. According to the considered low-Mach number approximation, the pressure is represented as a sum of thermodynamic pressure, which is assumed to be constant, and dynamic component of pressure fluctuations. To determine dynamic pressure a Poisson equation is solved at each time step. Herewith the value of velocity divergence is calculated from the equation for energy, taking into account both energy change due to heat release and heat transfer and the energy change according to the equation of state. To achieve detailed description of the simulated processes the thermal conductivity, multicomponent diffusion, natural convection and energy release due to chemical transformations were taken into account. Specific heat capacities and enthalpies of formation are calculated using the JANAF tables [2]. Diffusion model is based on the zeroth-order Hirshfelder-Curtiss approximation [3]. Mixture averaged transport coefficients were obtained from the first

principles of the gas kinetics theory [4]. Diffusion velocities were calculated taking into account the correction velocity approach proposed in [5]. Thermal diffusion and Soret effects were not incorporated into the model. Chemical kinetics was calculated according to the contemporary kinetic scheme [6].

RESULTS AND DISCUSSION

Let us first analyze the stability of the flame ball subjected to the buoyancy force immediately after ignition. After the mixture is ignited near the isothermal wall the main mechanism of the combustion is the diffusion of the deficient reactant, which is hydrogen in our case, to the reaction zone. Stability of this diffusive flame is determined by the heat loss to the cold isothermal wall [7]. As combustion proceeds, hot combustion products become involved in upward motion by the buoyancy force. That motion determines the formation of gas-dynamical convective flow that consists of toroidal vortex located in the region related to the flame kernel (see Fig. 2). Gas-dynamical vortical motion determines flame surface stretch and lateral extension. In the case of 6 vol% (and richer) mixture, this surface stretch leads to the cap-shaped flame structure formation, whose further evolution will be discussed later. In less reactive 5 vol% hydrogen (and leaner) mixture flame stretch results in flame surface local breakup in the stagnation point near vicinity of the flame surface. Kinetic energy dissipation into heat within vortical structures defines local temperature increase in this area that supports flame kernels located near the center of vortical motion. However, spatial scales of these kernels are not enough to maintain stable combustion. So, the reaction quenches finally.

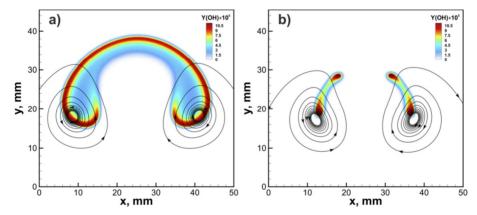


Fig. 2. Flame structure for time instant 180 ms after ignition. (a) mixture with hydrogen content 6 vol%; (b) mixture with hydrogen content 5 vol%. Background is colored by OH concentration.

One of the distinguishing features of the ultra-lean flame is the superadiabatic temperature of the hot combustion products which is due to the dominant diffusion mechanism of combustion. In microgravity conditions, the balance between the superadiabatic temperature of the flame on the one hand and heat losses, on the other hand, determines its stability. That defines lower lean flammability limit measured for ultra-lean flame balls than that predicted for planar adiabatic flames. The same mechanism is relevant for the flame in terrestrial gravity conditions where the temperature of ultra-lean flame combustion products is as well higher than adiabatic values. In terrestrial gravity conditions, an additional factor in the form of the flame stretch by the convective flows alters lower flammability limit, which however is still lower than that for the adiabatic flame (see Fig. 3). Thus flammability limit obtained for microgravity conditions in spherical symmetry is estimated as $\sim 4 \text{ vol}\% \text{ H}_2$, which is in good agreement with the leanest composition for which flame

balls were observed [1]. At the same time the flammability limit for the flame in terrestrial gravity is 5.25-5.50 vol% H₂ whereas adiabatic planar flame limit is 9 vol% H₂.

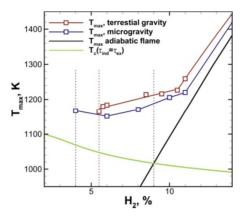


Fig. 3. Maximum temperature of the flame for various compositions of hydrogen-air mixture. Green line $-T_c$, crossover temperature; red line $-T_{max}$ for terrestrial gravity conditions; blue line $-T_{max}$ for microgravity conditions obtained from additional calculations in spherical symmetry; black line $-T_{max}$ for adiabatic flame. Dashed lines represent stable combustion limits for ultra-lean flames in microgravity conditions (dashed blue line), terrestrial gravity conditions (dashed red line) and freely propagating planar flame (dashed black line).

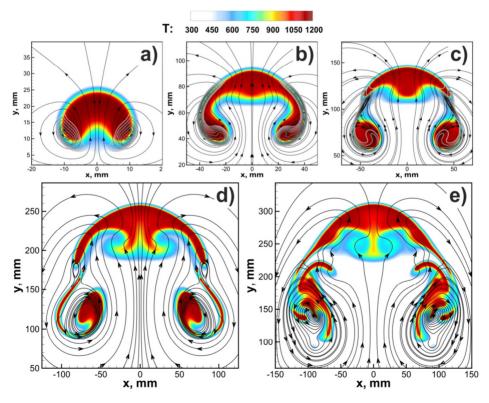


Fig. 4. Ultra-lean hydrogen flame evolution. (a) 100 ms, (b) 350 ms, (c) 500 ms, (d) 800 ms, (c) 950 ms. Background is colored by temperature. Streamlines are illustrated by the solid lines with arrows. On figures (a), (b), (c) vorticity contours colored by the vorticity are also presented.

After the initial stage, if the flame overcomes stretch induced by convection (e.g. in a mixture with hydrogen content 6 vol% and richer), the upward propagation caused by the buoyancy force continues. At the same time, the flame area becomes larger (see Fig. 4 a,b). Cap-shaped flame structure evolves and undergoes several breakup events due to the lateral flame surface detachment in recirculation area behind the main flame core (see Fig. 4 c,d). However, detached flame kernels do not quench and rise with the main core in its thermal wake. Due to a higher temperature in the wake, these kernels sometimes even reconnect with the main flame core. All these processes determine complex large-scale structure of the stable developed flame ball (see Fig. 4 e) which consists of the main flame core and several stable flame kernels moving behind it.

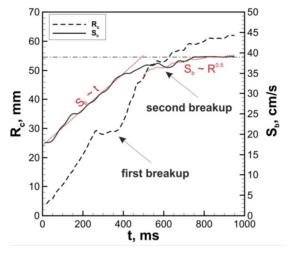


Fig. 5. Histories of the flame front leading point rising velocity (S_b) and curvature radius of the main flame core (R_c) . Theoretically predicted terminal velocity for the closed bubble with curvature radius 62 mm shown by dash-dotted horizontal line. Dashed red lines represent approximations of the rising velocity on different stages of flame development.

Evolution of the flame in the ultra-lean hydrogen-air mixture is similar to that of the gas bubble rising in liquid [8]. Gas-dynamical flows induced by the upward motion of the flame are also in good agreement with those developing during the bubble rising [9] and similar to the bubble with small values of the surface tension. In such a case high enough strain rates lead to the peripheral breakup of the flame structure [10]. Taking into account qualitative correspondence between two phenomena one can use theoretical estimations obtained for the closed bubble to describe flame-ball rising in the ultra-lean mixture under terrestrial gravity conditions. In particular, it is known that bubble achieves terminal rising velocity that can be estimated as $S_b = 0.5\sqrt{gR}$, where R is the curvature radius of the bubble [11]. Figure 5 shows histories of the rising velocity and the curvature radius of the main flame core measured near the symmetry plane. From Fig. 5 it is evident that flame core achieves terminal velocity $S_b \sim 38.9$ cm/s, that is in a good agreement with theoretical estimation for bubble terminal velocity. It should be noted that flame core terminal velocity is much higher than combustion velocity in the mixture of the considered compound.

CONCLUSIONS

Convective gas-dynamical flows accompanying the process of flame evolution in ultra-lean hydrogen-air mixtures in terrestrial gravity conditions play a crucial role on every stage of the flame development. Immediately after ignition convective flows determine stretch of the flame surface

that in the case of the near limit flames can result in the local breakup of the flame and subsequent flame quenching despite the superadiabatic temperature of the combustion products. As a result, lean concentrations limit for the stable flame formation in terrestrial gravity occurs to be greater compared with that measured in microgravity conditions but still lower than the limit for the adiabatic planar flame. Further development of the flame is governed by the convective rise of the hot combustion products and lateral expansion due to vortical flows. Obtained structure of the ultralean hydrogen-air flame represents the stable cap-shaped main core followed by the widely spread in space multi-kernel combustion zone. Stable large-scale structure of the flame propagating with the terminal velocity much greater than burning velocity in ultra-lean mixtures pose a threat for fire and explosion safety that should be taken into account in the development of safety measures.

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