Modeling of Laminar LOX/H_2 Flames in the Counterflow Configuration

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Abstract

The paper concerns structures of laminar LOX/H_2 spray diffusion flames in the counterflow configuration for high subcritical, cryogenic conditions. A model is presented that includes detailed transport and detailed chemical reactions which enables the investigation of both the inner flame structure and the extinction of these flames. The resulting information is not only interesting if laminar flame structures are to be investigated, moreover it may be used to simulate turbulent spray diffusion flames within a flamelet formulation. This enables the modeling of turbulent LOX/H_2 spray flames for conditions of cryogenic combustion.

Introduction

An improved understanding of the physical and chemical processes occurring in liquid rocket engines is required to ensure the stability, reliability, and efficiency of their performance. The gaseous hydrogen and the liquid oxygen (LOX) are injected at cryogenic inlet temperatures, and the turbulent combustion occurs both in the sub- and supercritical domain. Therefore, the models for the processes in systems such as the Ariane V or the Space Shuttle main engine are very complex. Experiments with LOX and hydrogen are extremely rare because of safety aspects. Thus, numerical simulations are very beneficial.

The combustion of LOX/H_2 takes place in the flamelet regime of turbulent combustion [1]. Therefore, the turbulent flame may be considered as an ensemble of laminar flamelets which are exposed to strain and curvature during the turbulent combustion process. The aim of this study is the numerical investigation of laminar stretched LOX/H_2 counterflow spray flames using both detailed chemistry and detailed transport for cryogenic temperatures and high subcritical pressures.

Model

A dilute LOX spray is considered that is injected with a gaseous hydrogen carrier versus hydrogen in the counterflow configuration. The present investigation concerns monodisperse sprays that are modeled using Lagrangian equations. However, the model is not restricted to monodisperse sprays [2]. The two-dimensional Eulerian gas phase equations are transformed into one-dimensional conservation equations using a similarity transformation [3, 4]. Source terms in the gas phase equations account for interaction with the liquid phase. The description of the gas includes a detailed chemical reaction mechanism [5] for the hydrogen/oxygen system that has been used in an earlier study of gas flames for pressures up to 10 MPa [6]. The gas phase transport coefficients are computed from the NASA polynomials which cover the temperature range between 300 and 5000 K. This set was extended by data from JSME tables [7] for the temperature range between 80 and 300 K and for pressures up to 20 MPa. Moreover, the pressure (and temperature) dependence of the vaporization rate and of the binary equilibrium composition at the liquid/gas interface [8] is included. Convective droplet heating and vaporization is formulated with a conduction limit model of Abramzon and Sirignano [9].

Results and Discussion

Figure 1 exemplarily presents the flame structure of a monodisperse LOX/H_2 counterflow spray flame at two different gas strain reates of 1,000/s (left part), and 3,000/s (right part), evaluated on the left side of the configuration. The initial spray and gas velocities are equal (1.054 m/s for the low strain rate



Figure 1: Flame structure with gas strain rates of a = 1,000/s (left), and a = 3,000/s (right).

situation), and their value increases proportional to the square root of the strain rate. The pressure is 3 MPa, the inlet temperature of hydrogen in both the streams is 100 K, and the initial LOX temperature is 80 K. The equivalence ratio on the spray side equals 10, and the droplets have an initial radius of $25 \ \mu m$.

Figure 1 presents the outer flame structure for both the conditions. Circles present both the size and position of the droplets. The increase of strain (right part) considerably decreases the flame thickness, and the droplets penetrate considerably deeper into the flame front. This is associated with the increased momentum of the droplets; the velocity profiles of both gas and liquid phase for both the conditions are shown in the lower part of Fig. 1. The figure shows that the increased momentum of large droplets causes a higher slip between the gas and droplet velocities.

The differences in droplet motion also affect the droplet vaporization, see the lower part of Fig. 1. The vaporization takes place in a broader regime that extends into the colder flame region. That droplet vaporization again drastically reduces gas temperature. In the area of reduced gas temperature, the combustion is reduced leading to lower values of H_2O compared to the lower strain rate situation. Another reason for the reduced values of H_2O , of course, is the elevated strain that reduces residence time of the reactants. In summary, the slower chemical reactions and the reduced residence time lead



Figure 2: Inner flame structure of the reaction zones on the spray side (left) and on the gas side (right) of the configuration for a = 3,000/s.

to the higher values of molecular oxygen shown in the right part of the figure.

Figure 2 displays the inner flame structure of the reaction zones on both the spray side (left part) and at the gas side of the configuration (right part) for the high strain situation of Fig. 1. The inner flame structure of the lower strain case is almost the same and not shown. Some profiles on the spray side of the configuration show a non monotonic behavior that is caused by vaporization (and therefore, it is not present in the gas diffusion flame on the gas side). Vaporization of course mainly affects the oxygen profile. On the one hand, gaseous oxygen is produced through vaporization and conversely, it is consumed through chemical reactions. In some regions of the flame, the one or the other process is more dominant leading to the profile shown in Fig. 2. A more detailed analysis may be found in Ref. [2]. The principal profiles of the species HO_2 and H_2O_2 follow that of the oxygen. These minor species are dominantly produced through reaction steps that include O_2 and its immediate reaction products (e.g. the OH radical).

An analysis of the net reaction rates of the most important elementary reactions for the production and consumption of HO₂ and H₂O₂ shows that HO₂ is mainly produced through the reaction step $H+O_2+M \Leftrightarrow HO_2+M$ and consumed through $HO_2+H \Leftrightarrow OH+OH$ where the absolute contribution of the latter reaction with respect to OH is of minor importance (leading to the smooth profile of OH shown in Fig. 2). The species H_2O_2 then is mainly produced through reaction $HO_2 + HO_2 \Leftrightarrow H_2O_2 + O_2$ in relatively cold regions of the flame (due to the stability of that species). As gas temperature increases, H_2O_2 is consumed in reaction $H_2O_2 + M \Leftrightarrow OH + OH + M$.

On the right side of the configuration where all droplets are completely vaporized, the components react in a pure gas diffusion flame. Non monotonic mole fraction profiles are not observed in the gas diffusion flame which confirms that the non monotonic behavior on the spray side is caused by droplet vaporization.

The gas phase combustion shows typical features of pure gas phase flames. Note that in both the combustion regimes of the flame (c.f. Fig. 2) the profiles of O and OH peak at the position where the gas temperature attains a local maximum. The peak of the H radical is shifted to the fuel side of the configuration, that is towards the boundaries of the configuration where pure molecular hydrogen enters the spray flame. The elevated level of concentrations in the zone between the two reaction zones is associated with the elevated level of strain and gas temperature in that flame.

The results shown here demonstrate that the flame structure of LOX/H_2 flames is strongly influenced by the vaporization process. Even some of the profiles of minor species are affected by the evaporation of droplets. As strain rate is increased, the flame is considerably narrowed, the droplets penetrate deeper into the flame, and the gas temperature is strongly reduced in the main vaporization zone. A further increase of strain eventually will lead to flame extinction which is currently under investigation.

Summary and Future Research

The structure of monodisperse LOX/H_2 spray flames in the counterflow configuration has been investigated by means of numerical simulation. A study of various relevant conditions are currently under investigation. It concerns a parameter study that includes variation of equivalence ratio towards leaner flames, pressure, droplet size and velocity as well as strain rate. In particular, extinction conditions are investigated.

The laminar flamelet structures will be included in a flamelet model for turbulent spray flames for comparison with experiments in systems such as the Mascotte and the micro combustion chamber M3.

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