CrossMark

Direct numerical simulation of lean premixed CH$_4$/air and H$_2$/air flames at high Karlovitz numbers

Henning Carlsson[*], *Rixin Yu*, *Xue-Song Bai*

Division of Fluid Mechanics, Lund University, 221 00 Lund, Sweden

ARTICLE INFO

ABSTRACT

Three-dimensional direct numerical simulation with detailed chemical kinetics of lean premixed CH$_4$/air and H$_2$/air flames at high Karlovitz numbers (Ka ~ 1800) is carried out. It is found that the high intensity turbulence along with differential diffusion result in a much more rapid transport of H radicals from the reaction zone to the low temperature unburned mixtures (~500 K) than that in laminar flamelets. The enhanced concentration of H radicals in the low temperature zone drastically increases the reaction rates of exothermic chain terminating reactions (e.g., H + O$_2$+M = HO$_2$ + M in lean H$_2$/air flames), which results in a significantly enhanced heat release rate at low temperatures. This effect is observed in both CH$_4$/air and H$_2$/air flames and locally, the heat release rate in the low temperature zone can exceed the peak heat release rate of a laminar flamelet. The effects of chemical kinetics and transport properties on the H$_2$/air flame are investigated, from which it is concluded that the enhanced heat release rate in the low temperature zone is a convection–diffusion-reaction phenomenon, and to obtain it, detailed chemistry is essential and detailed transport is important.

Introduction

Turbulent premixed flames have for a long time been a focus of research due to their extensive industrial usage, e.g., in gas turbines and internal combustion engines. At low intensity turbulence conditions, the structure of the flame is known to be similar to that of a laminar premixed flame. The flame is characterized by a multiple-zone structure: starting from the unburned mixture, a preheat zone, where there is no significant chemical reaction owing to low temperature, a reaction zone, where fuel is converted to combustion products, and finally a post-flame zone where temperature is high but the chemical reactions are in equilibrium. For hydrocarbon flames, the reaction zone can be further divided into a fuel consumption layer, which is also known as the inner layer, where fuel is converted to CO and H$_2$, and an oxidation layer downstream the inner layer, where CO and H$_2$ are further oxidized to CO$_2$ and H$_2$O [1,2].

For premixed combustion in a turbulent environment the flame structure is highly depending on the flame/turbulence interaction, which can be classified into different regimes [3] based on non-dimensional parameters such as Karlovitz number (Ka). The Karlovitz number is defined as the ratio

between the chemical time scale, τ_c, and the shortest turbulence time scale, the Kolmogorov time scale, τ_η. At high Karlovitz numbers, the Kolmogorov scale can be smaller than the chemical reaction time scale [3,4] and the small scale turbulence can disrupt the inner thin reaction layer, creating a distributed combustion region of broken and disconnected reaction zones. With the current trend, where many industrial combustion devices are pushed towards leaner operating conditions with subsequent thicker flames and lower laminar flame speed, the Karlovitz number in such applications tends to increase [5]. Very high turbulence intensity can be generated by high-swirl combustor nozzles, which are often used for flame stabilization in gas turbines. Stopper et al. [6] studied an industrial gas turbine burner, where Ka ~ 230 was obtained for a power output of ~1 MW. With increasing demand on power, the conditions of such swirl-operating gas turbines are pushed further into the distributed reaction zone regime. Strakey et al. [7] showed in measurements of an experimental swirl combustor that turbulence intensity of 150 times the laminar flame speed could be obtained (Ka ~ 600). Due to the existence of fine length and time scales in such flames it is difficult to resolve all these fine scales in either experiments or numerical simulations, and as such, the reaction zone structures at high intensity turbulence high Karlovitz number conditions are not well understood.

Turbulence/chemistry interaction is typically two-fold: on one hand it is well known that the chemical reaction can affect the flow field through gas expansion from heat release, on the other hand turbulence may also affect chemical reactions both indirectly and directly. Turbulence will typically induce an overall higher effective diffusion rate, which causes the mean structure to develop into a thickened flame brush with an increased mean flame speed; the chemical reactions are then adjusted indirectly to respond to the altered flame profile. Another mechanism of turbulence affecting chemistry may be by more direct disturbance of the chemical pathway through a sequence of elementary reactions. In a turbulent environment, the temperature field and the concentration fields of various major and intermediate species can be significantly different from the manifold of a laminar flame. For high Karlovitz number flames, such scattering may become large enough to cause the reaction to proceed through unconventional pathways.

A chemical kinetic mechanism, consisting of detailed elementary reactions, usually contains two groups of important reactions: the chain branching and chain termination reactions [8]. The chemical pathway can be affected by the balance between the chain branching and termination reactions; in a detailed chemistry mechanism, there may exist multiple chain branching/termination reactions. In case turbulence is intense, we may hypothesize (and as we will show later) that some of the species involved in (usually negligible) chain branching/termination reactions can be transported by rapid convection to a level to enhance/suppress those reactions. This effect we refer to as deviation from conventional chemical pathway. A goal of this work is to identify such change of chemical pathway in high Karlovitz number turbulent premixed flame. If the phenomena are verified, it is also important to understand through which elementary reaction such change proceeds and how such change will be affected by the use of different fuels, chemical kinetic mechanisms, and transport properties.

Previous studies of high Karlovitz number combustion systems have been performed with both experimental and computational approaches. Relying on planar laser induced fluorescence (PLIF) technique, several experimental works [9—16] have been performed for Karlovitz number around (and above) 100; most of these studies were aimed at identifying the effect of local quenching and reignition. For numerical studies of fundamental turbulent combustion processes, direct numerical simulation (DNS) [17—21], with the capacity of resolving the full turbulent flow spectrum, has gained increased popularity. Using simplified chemistry (with a model based on first order Arrhenius kinetics and a simplified reaction—diffusion model), Poludnenko and Oran [22,23] carried out three-dimensional (3D) DNS of a premixed H_2/air flame at Karlovitz number above 100; the work was focused on examination of the flame structures. To describe the details of the multiple reaction zone nature in flames, relatively detailed elementary reactions are needed; it is therefore essential to perform DNS studies with detailed chemistry. Few such studies have however been performed, due to the high demands on computational power and on robust/accurate numerical algorithm. The application of 3D-DNS with detailed chemistry is limited to combustion systems studying autoignition [21], premixed or partially premixed combustion at low Karlovitz number [24—26], and jet or shear layer flames [27,28]. A recent review on this topic is given by Chen [29]. For the study of premixed flames at high Karlovitz number, Aspden et al. [30—32] performed 3D-DNS to examine the effect of differential diffusion in flames of different fuels with detailed chemistry. Savre et al. [33] also performed a DNS study at high Karlovitz number in a two-dimensional (2D) configuration; the study was focused on the phenomenon of quenching/reignition. It should be noted that a detailed analysis of the balance between chain branching and termination reactions is performed in an early 2D-DNS work by Echekki and Chen [34], where the investigated combustion system is of autoignition type.

The above-discussed challenge is addressed in this work by performing the state-of-art 3D-DNS of turbulent premixed flames at high Karlovitz number with a detailed chemistry solver. This study focuses on the direct effect of turbulence on chemistry. Two different fuels are investigated in 3D configurations with a similar Karlovitz number: an H_2/air flame and a CH_4/air flame. While 3D-DNS is time consuming, we also perform additional 2D-DNS to examine the influence of the chemical kinetic mechanisms and transport properties. This article is organized as follow. The numerical method is described briefly in Section Numerical method. In Section Computational cases, the computational setup and the studied cases are stated. Section Results and discussion is divided into three parts, where the flame structure at the high Karlovitz number condition is firstly discussed. In the second part of Section Results and discussion, changes from conventional low Karlovitz number flames are investigated and analyzed in detail and in the last part of Section Results and discussion, amplified heat release rate due to the change in the flame structures is quantified. In Section Conclusions, the main conclusions of this work are given.