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Hydrogen-enriched non-premixed jet flames: Analysis of the flame surface, flame normal, flame index and Wobbe index

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ABSTRACT

A non-premixed impinging jet flame is studied using three-dimensional direct numerical simulation with detailed chemical kinetics in order to investigate the influence of fuel variability on flame surface, flame normal, flame index and Wobbe index for hydrogen-enriched combustion. Analyses indicate that the fuel composition greatly influences the H_2/CO syngas combustion, not only on the important local stoichiometric iso-mixture fraction surface distribution but also on the vortical structures in the flow field. As a result of CO addition to hydrogen-rich combustion, changes of the reaction zone in the flammable layer, shift of peak flame surface density distribution, shift of non-premixed regions, formation of widely populated scalar dissipation distribution rate with respect to tangential strain and reduction of global heat release are all found to appear. In particular, the CO addition induces a micromixing process which appears to be an important factor for the modelling investigation of turbulence/chemistry interaction especially for combustion modelling of H_2-rich syngas fuels.

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Introduction

Hydrogen-rich syngas combustion has received a great deal of interest in combustion technology over the past few decades as a potential future energy source of limiting atmospheric emissions of CO_2 in order to mitigate the global climate change [1–5]. In order to meet the ambitious targets for the reduction of greenhouse gas emissions, significant advancements in combustion technology for cleaner alternative fuels are required [6,7]. For this purpose, computational simulation is an essential tool which can accelerate the technology development by integrating numerical results with combustion theory thereby achieving a better understanding on the clean burning characteristics, which is the prerequisite for the development of clean combustion technology [8]. Direct numerical simulation (DNS) in which the complete spectrum of scales is resolved, produces realistic realisation of turbulent combusting flames which can potentially help to identify fundamental physical mechanisms of flame characteristics and turbulence/chemistry interactions [9–11]. The integration of DNS and theoretical formulations enables us to analyse the

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mechanisms in detail to reveal the underlying physics and therefore systematically link the information obtained from numerical simulations to combustion modelling theory to characterise chemically reacting flows.

There is a variety of theoretical analysis of non-premixed combustion available in the literature, e.g. Refs. [9–11], where the conserved scalar description of the flow field is often employed [12,13]. Vervisch and Poinsot [10] reviewed four different techniques for the analysis of DNS results of turbulent non-premixed combustion. The first is the flame surface analysis [14,15], which describes the dynamics and physical properties of iso-concentration surfaces. This analysis also provides evidence on the effects of turbulence on scalar mixing and therefore it can be used to develop modelling strategies in line with flame surface defined by the set of points on the stoichiometric surface of the mixture fraction which is a conserved scalar. The second is the flame normal analysis which describes the structure of the reacting flow in the direction normal to the flame surface and evaluates the curvature effects [10]. One-point scatter data analysis [16,17] and edge-flame analysis are also theoretical tools which can be used to study DNS data. In addition to these four techniques, there are other qualitative and quantitative tools that can be used to identify the mixing and heat release characteristics of combusting flows. Such tools can provide further insights into DNS results, which are particularly important with respect to diluted fuel mixtures. For example, Yamashita et al. [18] proposed analysis of the flame index defined as the degree of alignment of the fuel and oxidizer concentration gradients which distinguishes premixed flame from non-premixed flame in turbulent non-premixed jet flames. Flame index analysis has been employed in several DNS studies, not only to distinguish premixed flame from non-premixed flame but also to measure the mixedness of the flow [19,20]. The Wobbe index [21] which measures the amount of heat release by certain fuel or fuel mixture is defined in the specifications of gas supply particularly when fuel mixtures are burnt. It is used to compare the combustion energy output of different fuel compositions associated with variable fuel mixtures, which is a useful parameter in the understanding of the effects of fuel variability.

Besides the different types of flame analysis that can be performed using DNS, there is also a strong possibility of using DNS data to quantify the molecular mixing for the development of micromixing models which plays an important role in combustion modelling [22–24]. Since micromixing mechanisms acting at small scales bring reactants in contact within thin reaction zones, the choice of suitable parameters to describe the internal structure of the thin layers and their behaviour directly linked with the micromixing can be effectively mapped from the information rich DNS data [25]. Since the fundamental issue with syngas combustion is associated with the significant variation in their compositions that changes the molecular mixing, DNS results of syngas combustion can provide detailed information on the small scale mixing of turbulent flames that help to understand the mechanisms of micromixing with respect to fuel variability, which are complex and are not well characterised or understood particularly for the H_2-rich syngas fuels.

It remains a challenge to systematically extract information on flow physics from a large scale DNS database and analyse the flame dynamics such as the combustion characteristics of H_2 and H_2-rich syngas combustion, which is important to establish a fundamental understanding of the flame behaviour to facilitate the combustion model development for the prediction of combustion of cleaner fuels in practical applications. In addition, there is a scope for providing information based on DNS for micromixing phenomenon with respect to fuel variability. The present study is part of a larger effort to identify the flame characteristics of hydrogen and syngas combustion. For example, our previous investigations addressed several important research questions relevant to hydrogen and syngas combustion, which include formation of inner and outer vortical structures of hydrogen flame with the influence of buoyancy [26], near-wall heat flux of hydrogen flame with the influence of buoyancy [27], influence of fuel variability on flame dynamics of H_2/CO/CO_2/N_2 syngas flames for clean coal based integrated gasification combined cycle (IGCC) gas turbine combustion applications [28,29], effects of preferential diffusion on hydrogen and hydrogen-rich syngas combustion [30] and chemical species concentrations of hydrogen and hydrogen-rich syngas combustion [17]. The purpose of this study is to provide a comprehensive mathematical analysis of the fundamental combustion characteristics of H_2 and H_2-rich syngas non-premixed flames using four different types of theoretical methods and improve the current understanding of combustion induced micromixing process of cleaner fuels.

In the present study, DNS results of non-premixed impinging jet flames [30] were analysed using four different types of analysis methods: flame surface analysis [14,15], flame normal analysis [10], flame index analysis [18] and Wobbe index analysis. In this work, we considered an impinging jet flame configuration to fully explore the theoretical analysis and micromixing phenomenon of near-wall flame structure, where near-wall combustion is applicable to a range of practical industrial combustors such as gas turbine and internal combustion engines. The present paper begins with a brief description of the numerical implementation in Section 2. Theoretical analyses obtained from DNS data and modelling towards the micromixing are presented in Section 3. Finally, conclusions are drawn in Section 4.

Numerical implementation

DNS solves for all scales of the fluid motion and thus numerical solution of the governing equations must capture relevant scales of the fluid flow, chemical reaction, viscous dissipation and diffusion [10]. Simulations have been carried out using a parallel compressible DNS code [30] coupled with the flamelet generated manifold chemistry tabulation [31] for hydrogen-enriched combustion. The code solves the continuity equation, Navier–Stokes momentum equations, the energy equation, the mixture fraction equation, and the progress variable equation which accounts for preferential diffusion (non-unity Lewis number) effects, and the state equation for the fuel mixture. Details of the governing equations and flamelet generated manifold equations are reported elsewhere [26,30]. The spatial derivatives in all three directions are solved using a sixth-order accurate compact finite

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