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Large eddy simulation of fuel variability and flame dynamics of hydrogen-enriched nonpremixed flames

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ABSTRACT

In this study large eddy simulation (LES) technique has been used to predict the fuel variability effects and flame dynamics of four hydrogen-enriched turbulent nonpremixed flames. The LES governing equations are solved on a structured non-uniform Cartesian grid with the finite volume method, where the Smagorinsky eddy viscosity model with the localised dynamic procedure is used to model the subgrid scale turbulence. The conserved scalar mixture fraction based thermo-chemical variables are described using the steady laminar flamelet model. The Favre filtered scalars are obtained from the presumed beta probability density function approach. Results are discussed for the instantaneous flame structure, time-averaged flame temperature and combustion product mass fractions. In the LES results, significant differences in flame temperature and species mass fractions have been observed, depending on the amount of H_2, $N_2$and CO in the fuel mixture. Detailed comparison of LES results with experimental measurements showed that the predicted mean temperature and mass fraction of species agree well with the experimental data. The high diffusivity and reactivity of H_2 largely affect the flame temperature and formation of combustion products in syngas flames. The study demonstrates that LES together with the laminar flamelet model is capable of predicting the fuel variability effects and flame dynamics of turbulent nonpremixed hydrogen-enriched combustion including syngas flames.

1. Introduction

Rising concentrations of greenhouse gases (GHG) in the atmosphere associated with energy-related activities raise many challenges regarding present energy sources and use. Fundamentally, all fossil hydrocarbon resources are non-renewable, and thus it is vital to develop more effective and efficient ways to utilise these energy resources for sustainable development. Although the majority of world energy is supplied from the combustion of fossil fuels (petroleum, coal and natural gas), their dominant role in the GHG emissions such as carbon dioxide (CO_2) emissions necessitates the shifting towards a low carbon technology [1]. However, since worldwide energy consumption is expected to grow further, it is necessary to continuously supply fuel for energy conversion and in the meantime to control GHG emissions [2]. Search for cleaner and alternative energy sources for low carbon energy technologies has recently become a major research topic worldwide.

Clean combustion as a means of energy conversion with limited environmental impact has a great potential in addressing major challenges in reducing GHG emissions, in association with new energy technologies such as carbon capture and storage which is one of the most effective approaches to reduce CO_2 emissions [3]. As a result of interest in clean combustion, hydrogen (H_2) and syngas combustion (mainly mixture of H_2 and carbon monoxide CO) is receiving renewed and increased interest, as it can be flexibly generated from a wide range of solid fuels including coal, biomass and waste products [4] as well as from natural gas. Because of the large amount of resources available worldwide, especially coal in the U.S., Europe, and Asia, there is an interest in using hydrogen and syngas fuels to significantly cut GHG emissions. H_2 production from fossil fuels and biomass involves conversion technologies such as reforming (hydrocarbons, oil), gasification, and pyrolysis (coal/biomass), while other conversion technologies such as electrolysis and photolysis can possibly be used when the source of H_2 is water [5]. The synthesis gas or syngas is mainly a mixture of H_2, CO and N_2 with the exact compositions dictated by the type of fuel source (often fossil fuels, biomass or waste product) and the conversion technology used. The available hydrogen in syngas mixtures largely increases the rate of CO oxidation as radicals are propagated through faster hydrogen-related reactions [6,7]. Compared with hydrocarbon fuels, the higher diffusivity and reactivity of hydrogen may lead to a higher flame temperature in combustion. In clean energy technologies based on syngas combustion, the fundamental issue is associated with the significant variation in syngas compositions that can influence flame dynamics including flame temperature, combustion products etc. Therefore design and development of syngas combustion for future clean energy systems need careful

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Table 1
Flame conditions and compositions of the syngas fuels.

Case	Flame H	Flame HN	Flame HNC1	Flame HNC2
Jet diameter (mm)	3.75	8.0	7.72	7.72
Jet velocity (m/s)	296.0	42.3	45.0	45.0
H_2 %	100	75	30	10
N_2 %	0	25	30	60
CO%	0	0	40	30

consideration of the effects of fuel variability on the flame properties such as flame dynamics, ignition and extinction limits [8].

Numerical simulation has the potential of closing the gap between theory and experiment and enabling dramatic progresses in combustion science and technology. LES has emerged as a promising numerical tool to simulate turbulent combustion problems corresponding to laboratory and practical scale configurations [9,10]. In the computation of complex combusting flows, the unsteady three-dimensional (3D) nature of LES has many advantages for turbulence modelling over the classical Reynolds-averaged Navier–Stokes (RANS) approach. However, in combustion LES, the chemical reactions usually occur well below the resolution limit of the LES filter width and consequently modelling is required to predict the chemistry. Combustion models which have been successfully used in the RANS context have been extended to LES to create sub-grid scale combustion models. For example, several groups employed equilibrium chemistry as a LES sub-grid model for the chemical reactions and obtained reasonable predictions for the thermo-chemical variables for laboratory scale nonpremixed jet flames [11–13]. The steady flamelet modelling concept [14] has been widely used in combustion LES, because of its simplicity and ability to predict minor species. LES with steady laminar flamelet model has been successfully applied to simulate the laboratory scale nonpremixed bluff-body flames and agreements with experimental measurements were obtained [9,15]. However, the steady flamelet assumption is not strictly valid for flows with slow chemical and physical processes. The unsteady flamelet equations have to be used to account for such physical processes for nonpremixed jet flames [16]. The well known conditional moment closure model originally derived in the RANS context [17] has also been extended to LES and applied to nonpremixed flames [18]. The flamelet/progress variable approach, which has the potential to capture the local extinction, re-ignition and flame lift-off, has been

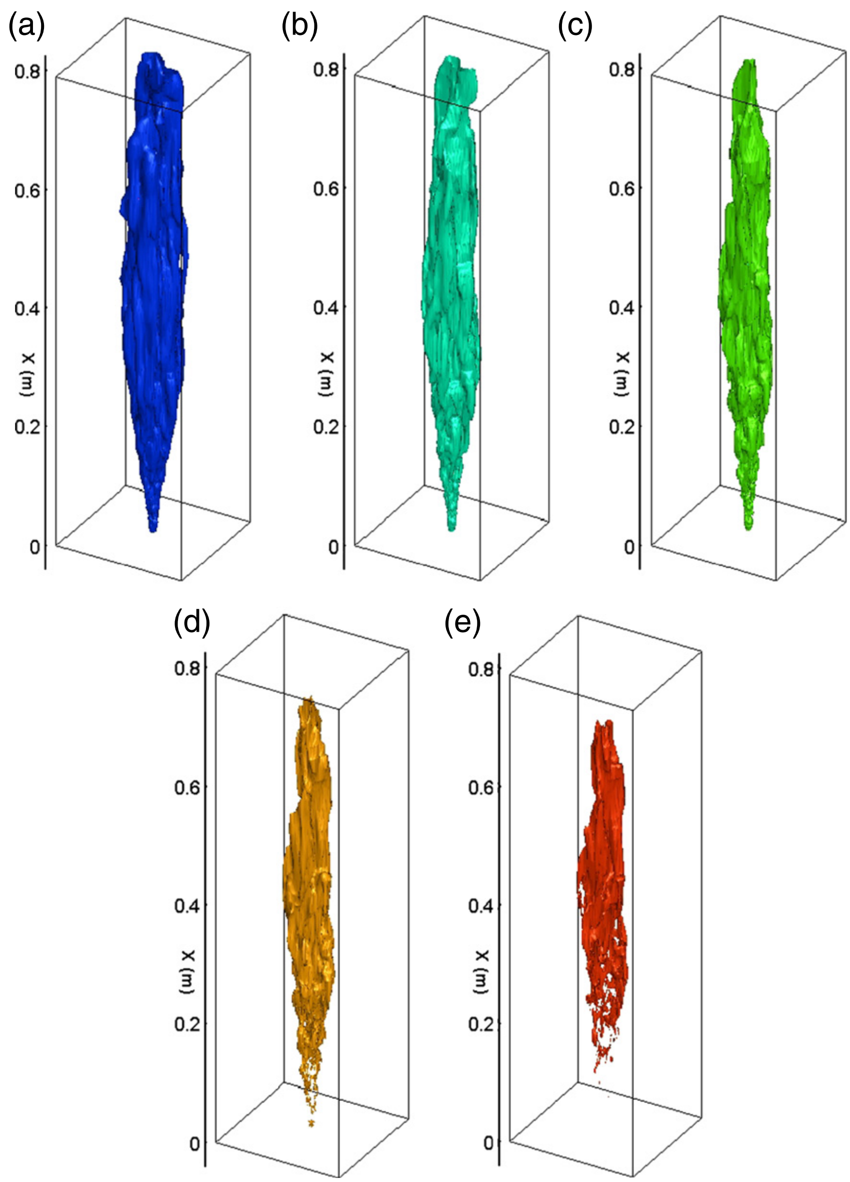

Fig. 1. Flame H: instantaneous three-dimensional visualisation of the flame temperature with iso-values of (a) T = 500 K, (b) T = 1000 K, (c) T = 1500 K, (d) T = 2000 K, (e) T = 2200 K obtained from LES calculation at t = 0.05 s.