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Differential molecular diffusion in a hydrogen-rich jet

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Abstract

Differential molecular diffusion effects are expected to be of particular importance in the combustion of hydrogen and H_2-enriched fuels. The mixing between fuel and oxidizer can be significantly influenced, implying changed chemical reaction rates and overall heat release. Here, the LEM3D model based on the Linear Eddy Model (LEM) is employed to simulate differential diffusion effects in a turbulent round jet of H_2 and Freon 22 issuing into air. Input to LEM3D, generated from ANSYS Fluent, consists of velocity profiles and profiles for the turbulent diffusivity, the Kolmogorov scale and the integral length scale. In this paper, the LEM3D-Fluent coupling is demonstrated by a coarse steady-state RANS simulation in Fluent with a one-to-one correspondence between the RANS grid cells and the LEM3D control volumes. The LEM3D simulation results are compared with previously obtained measurements of differential molecular diffusion for the given flow configuration.

Keywords: differential diffusion; hydrogen; turbulent combustion; turbulent mixing

1. Introduction

The combustion of hydrogen and H_2-rich fuels is a key part of the pre-combustion CO_2 capture concept. Great challenges must be overcome, however, in order to implement the burning of such low-carbon fuels in modern gas turbines. These challenges are linked to the distinct thermo-physical properties of hydrogen, such as a very high flame speed, wide flammability limits, and a higher diffusivity than any other gas. This leads to a dramatically

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different combustion behavior of hydrogen compared to conventional hydrocarbon fuels. Thus, the primary technology for low-NO_x power generation in stationary gas turbines, lean-premixed (LPM) combustion, is not yet developed for hydrogen combustion. Issues related to auto-ignition, flame stabilization, flashback, and NO_x control need to be resolved in order to achieve a clean, efficient, and safe burning of H_2-rich gases.

High-fidelity and reliable numerical design tools are essential keys to the development of novel combustor technologies pertinent to the use of fossil fuels and carbon capture. The numerical simulation tools, which are of great aid to the designers of new configurations, must be able to give accurate predictions of the mixing and reactions in the turbulent reactive flows. State-of-the-art simulation tools, based on the Reynolds Averaged Navier-Stokes (RANS) equations, rely on detailed modelling yet for the most part can only give a bulk approximation to the fluid flow and combustion processes. The reason is the lack of spatial and temporal resolution in the conventional RANS methods, which, due to the huge computational cost involved in detailed turbulent combustion processes, employ turbulence and mixing models that rely on the large-scale characteristics of the turbulent flow. State-of-the-art combustion models therefore have limited predictive capabilities in many practical engineering applications.

With the development of enhanced computational power, direct numerical simulation (DNS) of combustion processes for targeted canonical cases has become feasible [1]. DNS is based on first principles in its description of the fluid flow and the numerical resolution of the flow field is such that no model is needed for the turbulence-chemistry interaction. Previous DNS of non-premixed [2] and premixed [3] hydrogen flames have provided detailed information about the flow structures and turbulence-chemistry interactions in flame stabilization and flashback for gas turbine combustors. A DNS for complete combustor geometry is not feasible, however, and will remain so into the foreseeable future. Despite the limitations of DNS, the approach gives detailed insight into the combustion processes that can aid modellers as well as designers in their further work.

Due to the huge computational cost associated with DNS, alternative methods to provide small-scale resolution have been pursued in recent years. 1D approaches like the Linear Eddy Model (LEM) [4] and the One-Dimensional Turbulence (ODT) model [5] are methods that resolve all scales of turbulent reactive flows at a computationally affordable cost and with promising results [6-8]. In the present study we employ a novel formulation called LEM3D [9,10] to simulate the effects of differential diffusion in a hydrogen-rich turbulent jet. In LEM3D, small-scale resolution is provided by three orthogonally intersecting arrays of 1D LEM domains. LEM3D thus provides small-scale resolution in all three spatial directions of the turbulent flow field, and is by construction applicable as a sub-grid scalar closure both for RANS and Large Eddy Simulation (LES) applications. As a sub-structure for a global flow solver, LEM3D provides small-scale resolution at a computationally affordable cost compared to a corresponding DNS.

In the present work, LEM3D simulation results are compared with measurements from a previous experimental study of differential molecular diffusion in a turbulent round jet [11,12]. The measurements were performed in a turbulent jet of 90% H_2 and 10% Freon 22 (on a molar basis) issuing into air with jet Reynolds number 20,000. In the non-reactive experimental study, the effect of differential diffusion was isolated from the added complication of chemical reaction and heat release in a hydrogen jet flame. A detailed description of the experimental setup for measuring differential diffusion in the hydrogen-rich turbulent jet has been given by Dibble and Long [13]. Interesting effects that were observed experimentally have previously been interpreted qualitatively using 1D LEM [14]. That LEM formulation involved some specialized features needed to represent the specific flow geometry, including the introduction of cylindrical geometry on the 1D domain in a non-conservative way. We here apply LEM3D to a flow configuration that resembles the experimental setup. In a previous study, salient features of the measured results were reproduced qualitatively [15]. In the current work, local variation of the smallest eddy size has been incorporated, which represents an important extension of LEM3D towards the targeting of future applications to hydrogen-rich combustion and other low-emission combustion technologies. In addition, input profiles are here generated from ANSYS Fluent. In previous work [9,15], self-similar profiles generated on the basis of jet velocity and turbulence measurements were used as model input to LEM3D.

2. Differential diffusion

The effects of differential diffusion in turbulent jet flames of hydrogen have been recognized for a long time [16,17]. It has also been proposed, supported by LEM simulations and scaling analysis, that the decrease of these