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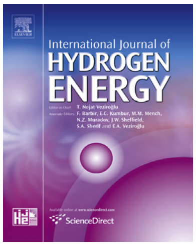

Numerical assessment of subgrid scale models for scalar transport in large-eddy simulations of hydrogen-enriched fuels

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ABSTRACT

A comparison of two different models addressing the scalar transport in large-eddy simulations is conducted for a non-reacting jet and an experimental flame. A simple approach based on a gradient diffusion closure is compared against the linear-eddy model in the context of hydrogen-enriched non-reacting fuel jets and flames burning hydrogen-enriched mixtures. The results show that the gradient diffusion model is not valid as a subgrid scale model for large-eddy simulations of mixtures containing hydrogen. It produces unphysical scalar fields with unrealistic temperature distributions. Approaches based on the linear-eddy model can be used instead to obtain appropriate representation of the scalar field and more accurate predictions of the scalar transport and the temperature field.

Introduction

The addition of hydrogen into fuel mixtures is becoming a common practice for cleaner energy conversion in applications involving the burning of practical fuels in combustion devices. The presence of hydrogen may reduce the formation of CO, CO_2 and NO_x, extend the flammability limits and increase the combustion efficiency [1]. However, issues such as flashback [2] or flame instabilities [3] could arise when these fuel mixtures are burned in practical systems due to the nature of the hydrogen compound. Hydrogen is very light and buoyant as well as highly diffusive and weakly viscous. These properties make this compound very different from traditional hydrocarbon fuels and its content in the fuel mixture affects the combustion dynamics to a large extent [4,5]. Among other fuels, syngas mixtures, which are mainly composed by hydrogen and carbon monoxide, are of particular interest because of their application in systems with low emissions such as the integrated gasification combined-cycle (IGCC) power plants [6]. Accordingly, investigation of these fuels and their combustion characteristics is of fundamental importance to the development of IGCC technologies [7].

Although the combustion of traditional hydrocarbon-based gas fuels such as methane, ethane or natural gas has a more complex chemistry than that of hydrogen [8], there are

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similarities between the dominant species governing the combustion process. Therefore, the formulation of models for combustion of hydrocarbon fuels might be based on overall properties of species such as constant Schmidt, Prandtl or Lewis numbers to reduce the complexity of the problem [9]. However, there exist some uncertainties in the applicability of traditional models when modelling the dynamics of hydrogen-enriched fuels because of the large differences found in the transport and chemical properties between the individual components of the mixture. Numerical simulations can provide insight into the physics of such mixtures provided that the models employed to obtain the flow fields are validated and the results correlate with the experimental data.

Large-eddy simulation (LES) may be an attractive method to simulate combustion of hydrogen-enriched mixtures for industrial applications [10,11]. LES is a numerical approach developed to simulate complex engineering flows by computing the large turbulent structures of the flow [12]. In LES, the large scales of the fluid motion are resolved by governing equations, while the effects of the small scales on the resolved fields are modelled using closure rules. This is performed by filtering the flow field in space and providing appropriate models for the subgrid scale terms. For the modelling of small scales, many subgrid modelling closures have been proposed in the literature.

General approaches following the Kolmogorov's universal inertial-range scaling theory are traditionally used to model the subgrid scale momentum transport [13]. As the small scales are mainly dissipative, gradient diffusion models based on the turbulent or eddy viscosity are often applied to account for their effects [14]. Although more sophisticated models based on scale similarity [15], the subgrid scale turbulent kinetic energy [16] or multifractal modelling [17] are also possible, gradient diffusion approaches have demonstrated to be suitable for general applications [18]. Nevertheless, analogous formulations based on gradient diffusion approaches could prove to be fairly poor on modelling the subgrid scalar transport [19]. Eddy diffusivity models assume that the subgrid flux aligns with the maximum scalar gradient and the accuracy of the models is compromised when this condition is not satisfied [20]. Despite other models were developed based on different concepts such as scale similarity [21] or stretch-vortex stresses [22], their applicability for reacting flows with heat release and differential transport phenomena is not yet demonstrated.

Furthermore, in combustion applications, the effects of molecular diffusion and turbulent stirring are crucial to represent precisely the mixing process of reactive flows. These two processes occur at molecular level below the LES resolution and play a determinant role in the entire combustion process. Thus, the subgrid scale models are required to provide a precise representation of the scalar field at the subgrid level in order to be suitable to represent reacting scalar fields. One of the major concerns of modelling hydrogen-enriched combustion is to account for the effects of differential and counter-gradient diffusion [23–25]. Although such effects may be modelled in a way coupled to the eddy diffusivity concept under certain conditions [26], generic models including mixing and transport properties of the species should be adopted for more general applications [27]. The linear-eddy model (LEM) proposed by Kerstein [28] is formulated to specifically account for the individual processes governing the mixing and reaction of turbulent reactive flows [24,29] and this approach is investigated here in the context of hydrogen mixtures. In LEM, the diffusion problem is deterministically treated by solving a governing equation and the effects of turbulence are considered using a stochastic approach [27]. LEM has been found to be adequate to describe the mixing problem when it is used as a subgrid scale model in LES [30]. Because differential and counter-gradient diffusion of chemical species is automatically accounted for in this model, LEM may prove to be a suitable technique to describe the mixing in hydrogen-enriched fuels.

The objectives of the present work are to test and validate two different approaches to model the scalar transport in LES for combustion applications of hydrogen-enriched fuels. This paper is organized as follows. The next section introduces the mathematical modelling and the physical problem addressed here. The computation of the budgets of the energy equation is also detailed in that section, which will be subsequently used to analyse the temperature distribution. Then, results of numerical simulations of non-reacting flows are presented with emphasis on the contribution of the energy budgets, where an abnormality in temperature distribution was observed. A discussion on the main differences between the predictions of the scalar fields by the two models is carried out subsequently. The results of the reacting case are compared against experimental data and some conclusions are drawn at the end.

Mathematical modelling

The LES equations presented here correspond to the Favre filter-averaged governing equations for reactive flows and include the conservation of total mass, momentum, energy and reactive scalars respectively. A box filter defined as $\Delta = V^{1/3}$ is employed to filter the equations in space, where V represents the cell volume. The notation '$\overline{\cdot}$' is used for quantities filtered in space and '$\tilde{\cdot}$' for Favre-averaged variables following $\tilde{f} = \overline{\rho f}/\overline{\rho}$. As two different approaches are considered to model the transport of species, these equations are presented in a separate subsection. The two models being compared are referred to as LES-EDC when the eddy diffusivity concept is used to model the subgrid scalar transport, and as LES-LEM when the linear-eddy model is employed instead.

Governing equations

The system of governing equations including the continuity, momentum and energy equations is given by:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \left(\overline{\rho} \tilde{u}_j \right)}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \left(\overline{\rho} \tilde{u}_i \right)}{\partial t} + \frac{\partial \left(\overline{\rho} \tilde{u}_j \tilde{u}_i \right)}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\tau}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} \tag{2}$$

$$\frac{\partial \left(\overline{\rho} \tilde{e} \right)}{\partial t} + \frac{\partial \left(\overline{\rho} \tilde{u}_j \tilde{e} \right)}{\partial x_j} = -\overline{p} \frac{\partial \tilde{u}_j}{\partial x_j} - \frac{\partial \overline{q_j}}{\partial x_j} + \overline{\tau}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial h_j^{sgs}}{\partial x_j} + \Theta^{sgs} + \overline{\dot{Q}^c} \tag{3}$$

where ρ, t, u_i, x_i, p, τ_{ij}, e, q_i and $\dot{Q}^c$ are the density, time, ith velocity component with $i = 1, 2, 3$, ith Cartesian coordinate,