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A two-equation model for non-unity Lewis number differential diffusion in lean premixed laminar flames

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ABSTRACT

Premixed flames are prone to develop thermo-diffusive instabilities when the diffusivity of the fuel is different from the rest of the mixture. Even when a uniform premixed composition is used, the local equivalence ratio across a flame front will not be constant. Therefore, a single quantity such as the progress variable is incapable of modeling accurately the combustion of non-unity Lewis number flames. In this work, a two-equation model is presented for the simulation of premixed laminar flames with non-unity Lewis number fuels. This model relies on the progress variable approach, which is suited for modeling premixed flames in which the fuel's Lewis number is near unity. An additional transport equation for a mixture fraction is derived for non-unity Lewis numbers. The model is verified to be consistent with simple laminar unstretched premixed flames. Hydrogen- and propane–air mixtures are used to demonstrate the model's ability to capture the respectively unstable and stable properties of each lean mixture. One dimensional spherical simulations reproduce the effects of flame stretch due to flow strain rate and flame curvature. Finally in two dimensions, the model captures the creation of cellular structures for negative Markstein length flames and the stable propagation of positive Markstein length flames.

1. Introduction

The combustion of lean hydrogen premixed flames in turbine burners is promising because it is characterized by low emissions and high efficiency [1]. However, the reacting flow induced by burning hydrogen presents significant technical and engineering challenges. As the hydrogen/air mixture approaches the lean flammability limit, the resulting combustion is subject to thermo-diffusive instabilities which might lead ultimately to unstable combustion, flashback, blow-off, and noise [2].

In complex large scale flows, the preferential diffusion due to hydrogen's non-unity Lewis number leads to local variations in equivalence ratio. Regions with leaner mixture burn slower, and regions with richer mixture burn faster. These instabilities, not specific to turbulent flows, originate at very small scales and may lead ultimately to large scale coherent structures. Such instabilities are also found in rich hydrocarbon flames [3].

Due to the inherent cost of performing numerical simulations of turbulent reacting flows, reduced order models need to be developed and these models should capture the differential diffusion effects. Several strategies for modeling large scale turbulent premixed flames have been developed. One such strategy consists of thickening the flame front by enhancing molecular diffusion [4,5]. This thickened flame model has the ability to describe a representation of the flame front on a coarse grid. However, the entire structure of the flame is lost, and small scale variations in equivalence ratio are damped out by the enhanced diffusion. Transported PDF methods [6,7] are another interesting strategy because they can be used in conjunction with detailed chemistry. However, the quality of this approach relies strongly on the quality of the micro-mixing model used, and the analysis of differential diffusion in the framework of transported PDF methods remains an open research question [8]. Several other strategies have been developed to reduce the cost of the numerical simulations and the modeling of the detailed chemical processes. Successful approaches include methods like FPI (flame prolongation of ILDM) [9] and FGM (flamelet generated manifolds) [10]. In these approaches, the flame properties and chemical source terms are mapped onto a single scalar referred to as the progress variable. These methods have been very successful at describing the combustion of fuels with close to unity Lewis number. However, lean hydrogen and rich hydrocarbon premixed flames with local variations in equivalence ratio cannot be described entirely

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and uniquely with a single scalar. For instance, previous studies have suggested using the fuel mass fractions as an additional scalar [11,12] or using element mass fractions (Y_H, Y_O, Y_N) as additional coordinates [9,12]. In more recent work [13], Bastiaans and Vreman supplemented conservation of mass and momentum with transport equations for temperature and the complement of the scaled hydrogen mass fraction. Simulations with this chemistry tabulation lead to the successful formation of cellular structures.

The first step towards capturing the differential diffusion effects in large scale turbulent flames is the development and validation of a simple, reduced order model for premixed laminar flames. The goal of this paper is to (1) propose such a model that captures the differential diffusion that occurs in lean premixed combustion of non-unity Lewis number fuels, (2) verify it captures global quantities such as flame speed, flame thickness, and mixture fraction variations in unstretched laminar flames, and (3) analyze the effects of flame stretch (curvature) on the flame propagation speed.

The present work is based on the Flamelet Progress Variable (FPV)-levelset approach developed by Knudsen and Pitsch [14,15]. The Flamelet Progress Variable (FPV) model was developed originally by Pierce and Moin [16,17] to represent non-premixed combustion and extended later by Ihme et al. [18,19]. In the combined FPV/Levelset approach, transport equations for three independent scalars are solved: mixture fraction (Z), progress variable (C), and levelset (G)

$$\partial_t(\rho Z) + \nabla\cdot(\rho\mathbf{u}Z) = \nabla\cdot(\rho D\nabla Z), \tag{1}$$

$$\partial_t(\rho C) + \nabla\cdot(\rho\mathbf{u}C) = \nabla\cdot(\rho D\nabla C) + \dot{\omega}_C, \tag{2}$$

$$\partial_t(G) + \mathbf{u}\cdot\nabla G = \frac{\rho_u}{\rho}S_L. \tag{3}$$

All relevant chemical properties are assumed to depend only on mixture fraction (Z) and progress variable (C) and are mapped into the flow field as $\phi = \phi(Z,C)$. The model accurately describes how the burning velocity (S_L) and chemical source term ($\dot{\omega}_C$) change with respect to changes in local equivalence ratio. In the case of fully premixed conditions, the mixture fraction remains constant, and the model depends only upon the progress variable and the levelset. The levelset was introduced in order to provide a more accurate and more robust tracking of the flame front in turbulent settings. Since the current work is focused on laminar flames, the levelset is not used and the reaction zones are fully resolved.

The objective of this paper is to present an extension of this model that relies on the mixture fraction to capture the differential diffusion inherent in non-unity Lewis number combustion. Lean premixed hydrogen- and propane–air mixtures will be used to test the model's ability to qualitatively capture the physics that characterize these flows. The focus of the present work is not to provide an extensive comparison and validation against experimental data, but to formally derive the model and to demonstrate its potential as a simple low-cost model that may eventually be applied to turbulent flows.

The article is organized as follows. In the first section, we derive mathematically a mixture fraction equation source term that appears when differential diffusion effects are considered. Then, a model for this source term is formulated and verified in simulations of 1D laminar unstretched premixed flat flames. An analysis of the model's response to flame curvature and strain rate and their effects on the laminar burning velocity is conducted in one dimension. Finally, two-dimensional simulations of perturbed planar flames demonstrate the unstable/stable propagation of hydrogen- and propane–air mixtures, respectively.

2. Extension to non-unity Le combustion

In non-unity Lewis number combustion, the local mixture fraction is not a conserved scalar because of the presence of differential diffusion. In this section a derivation is presented that extends the FPV approach [14,15] (Eqs. (1) and (2)) to account for local variations in mixture fraction. It begins with a demonstration of the mixture fraction variation that occurs with non-unity Lewis number for laminar unstretched premixed flames of hydrogen- and propane–air mixtures. Conditions used in these flames are consistent throughout the article. Next, the modeling assumptions are stated for the derivation. The diffusion flux is derived using these assumptions and is used to derive a modified mixture fraction equation with an additional source term. The section concludes with a discussion of chemical table creation and the unique mapping of chemical states onto Z–C space.

2.1. Mixture fraction variation

Figure 1 shows the profiles of mixture fraction (its exact definition will be given later, Eqs. (18)–(20)) and progress variable across laminar unstretched lean hydrogen- ($\phi = 0.4$) and propane–air ($\phi = 0.6$) premixed flames. These flames were simulated with the FlameMaster program [20] using detailed chemistry. The mechanism used for hydrogen–air mixtures may be found in Ref. [21] and that for propane–air mixtures was GRI-Mech 3.0.

Table 1 lists the Lewis numbers of the major global chemical species for both hydrogen- and propane–air flames. The Lewis number for oxygen is within 10% of unity for each fuel. The combustion products H_2O and CO_2 are within 20–30% of unity, respectively. The fuel species H_2 and C_3H_8 vary by as much as factors of two or three, respectively, which are notably larger deviations from unity Lewis number than any of the other species.

It is common for methane–air flames to be modeled as equidiffusion flames. In order to capture the instability introduced through differential diffusion, at least one species must have a non-unity Lewis number. In the approach that will be proposed here, the Lewis number of all species except the fuel is set to unity. In hydrogen–air mixtures the Lewis number is $\mathrm{Le}_{H_2} = 0.3$ and in propane–air mixtures $\mathrm{Le}_{C_3H_8} = 1.8$. These values are representative of the upper and lower range of Lewis numbers that are found in turbulent reacting flows.

The progress variable is defined as the mass fraction of water (H_2O) for hydrogen–air mixtures and the sum of H_2O, CO and CO_2 mass fractions for propane–air mixtures. As expected this variable increases across the flame front. Figure 1 shows that, because differential diffusion is present, the mixture fraction is not constant. The hydrogen–air flame's mixture fraction decreases near the flame front as hydrogen is transported towards the burnt side of the flame. In the propane–air flame, the mixture fraction increases across the flame because the fuel diffuses slower than the oxidizer. After the flame front, the mixture fraction returns to its initial, unburnt value as all diffusion terms go to zero.

2.2. Modeling assumptions

The variable mixture fraction profile in Fig. 1 is a result of a complex balance between diffusion and chemical reactions, which leads ultimately to a source term ($\dot{\omega}_Z$) in the mixture fraction equation (Eq. (1)). To derive this source term, we consider the following assumptions:

- one-step irreversible chemical reaction,

$$\nu_F F + \nu_O O_2 \rightarrow \nu_P P, \tag{4}$$