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A flamelet analysis of the burning velocity of premixed turbulent expanding flames

J.A. van Oijen*, G.R.A. Groot, R.J.M. Bastiaans, L.P.H. de Goey

Mechanical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

Abstract

Direct numerical simulation is a very powerful tool to evaluate the validity of new models and theories for turbulent combustion. In this paper, direct numerical simulations of spherically expanding premixed turbulent flames in the corrugated flamelet regime are performed. The flamelet-generated manifold method is used to deal with detailed reaction kinetics. The numerical method is validated for both laminar and turbulent expanding flames. The computational results are analyzed by using an extended flame stretch theory. It is investigated whether this theory is able to describe the influence of flame stretch and curvature on the local burning velocity of the flame. If the full profiles of flame stretch and curvature through the flame front are included in the theory, the local mass burning rate is predicted accurately. The influence of several approximations, which are used in other existing theories, is studied. When flame stretch is assumed to be constant through the flame front or when curvature of the flame front is neglected, the theory fails to predict the local mass burning rate.

Keywords: Turbulent premixed flames; Flamelets; Burning velocity; Reduced chemistry

1. Introduction

The development of accurate and efficient models for turbulent premixed combustion is one of the most challenging tasks facing the combustion community today. A major part of the current activities is based on the laminar flamelet concept, in which the idea is used that the chemical time scales in the flame are generally much smaller than those in the turbulent flow. This idea leads to the introduction of a flame front as a thin layer propagating through the surrounding flow field, while the turbulent eddies are larger than the flame thickness. A classification of the different available models for premixed turbulent combustion has been recently presented by Peters [1]. The oldest and most well-known model has been developed over the years by Bray and Moss [2] and is based on the assumption that the flame front is infinitely thin. Other interesting and promising models are the coherent flame model [3,4] and the G-equation model [1].

One of the most important ingredients of all flamelet models is the description of the influence of flame stretch and curvature on the behavior of the flame. Flame stretch and curvature effects on the one hand are responsible for the creation and destruction of flame surface area [4] and flame wrinkling [1]. On the other hand, it is well known that flame stretch and curvature have an important influence on the local mass burning rate of the thin instantaneous flame front. There are several ways to account for this influence into account, e.g., by using models derived from direct numerical

* Corresponding author. Fax: +31 40 2433445.
E-mail address: J.A.v.Oijen@tue.nl (J.A. van Oijen).

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simulation (DNS) data, measurement data or data arising from asymptotic theories. For instance, in the coherent flame type model ITNFS [5], the influence of stretch and curvature due to the turbulent structures in the flow is included in terms of a model based on DNS results of flames interacting with vortical structures. In case of the G-equation, the weak-stretch limiting behavior found in asymptotic methods is used [1]. It is doubtful, however, whether the weak-stretch theories available today can be used for the highly stretched turbulent flames in the corrugated flamelet and thin reaction zones combustion regimes.

de Goey and ten Thije Boonkkamp [6], however, introduced a new extended flame stretch theory recently. It is the aim of this study to evaluate whether this theory and simplified versions of it, including the asymptotic versions, are able to describe the influence of flame stretch and curvature on the local burning velocity in a turbulent flame. This study is carried out using DNS of spherically expanding premixed turbulent flames in the corrugated flamelet regime. DNS is a very powerful tool today to test the validity of new models and theories, and it has been very helpful in the evaluation of the different models mentioned above [7]. The current study focusses on the influence of local flame stretch and curvature fields on the local mass burning rate, for which a consistent picture is still missing today (see, e.g. [8]). The disadvantage of using three-dimensional (3D) DNS models is that the application of detailed chemical kinetic mechanisms is still limited. For this reason, we use the recently developed chemical reduction technique, referred to as the flamelet-generated manifold (FGM) method, to model the chemistry in the flame [9]. To be able to focus on the direct effects of stretch and curvature and to avoid that the results are obscured by related effects due to preferential diffusion, we restrict the analysis to unity Lewis numbers, in this study. Furthermore, unlike other studies, this research is based on DNS of highly curved spherically expanding turbulent flames, occuring, e.g., in spark-ignition engines. Although these flames are very relevant in practice, they have been scarcely studied (see, e.g. [10]) in the literature, probably because of the difficulties encountered to handle the open non-reflecting boundary conditions encountered with these simulations.

In the next section, the numerical approach of the DNS computations is described, including the boundary conditions, the initial conditions, and the FGM method. A validation of the model based on spherically expanding flames in both laminar and turbulent flows is presented as well. The basic flamelet theory and some modifications, which are used in the present study to analyze the DNS data in terms of the influence of stretch and curvature on the local mass burning rate, are summarized in the following section. Results of this analysis are also presented there. The paper is finished with a discussion in the last section.

2. Numerical approach

Freely expanding flames are modelled in a turbulent flow field by using DNS. In this section, the DNS calculations are described. More detailed information about the DNS program can be found in [11].

The fully compressible combustion equations are solved in a cubic three-dimensional computational domain with a length of 5.0 mm and 127 grid points uniformly distributed in each direction. This implies that the mesh size is approximately 0.04 mm in each direction. For the spatial discretisation of the equations, a compact finite difference method [12] is employed, which is sixth-order accurate. The time integration is performed with a compact storage third-order Runge–Kutta method [13]. Furthermore, parallel computing is implemented through OpenMP on a silicon graphics multi-processor platform.

The boundary conditions are modelled with the Navier–Stokes characteristic boundary conditions (NSCBC) [14]. Flames in an open environment are simulated, which means that all boundaries of the cubic computational domain have to be modelled as outlet boundaries to prevent pressure build-up in the domain. Therefore, non-reflecting outlet boundaries are required, which means that the gases are able to leave the domain and that the acoustic waves are not reflected at the computational boundaries. However, prescribing all boundaries as perfectly non-reflecting outflow boundaries can lead to an ill-posed problem because the mean pressure of the flow is not determined. The solution proposed by the NSCBC method is to use partially non-reflecting boundary conditions by implicitly imposing the pressure at infinity by the specification of incoming acoustical waves [14]. In this way, information about the mean pressure is allowed to travel from regions far outside the computational domain to the inside of the domain.

A stoichiometric methane–air mixture is considered at atmospheric pressure with an unburned temperature $T_u = 300$ K. The gas mixture is assumed to behave as a Newtonian fluid. Therefore, the viscous stress tensor is modelled with Stokes' law of friction [15]. The viscosity of the mixture is computed with Sutherland's theory [15], and the thermal conductivity over the heat capacity at constant pressure λ/c_p is assumed to be a function of temperature only [16]. The species heat capacities are tabulated in polynomial form. Unity Lewis numbers are assumed for all species to prevent that preferential diffusion effects obscure the direct effects of stretch and curvature on the mass burning rate.