Combustion and Flame 161 (2014) 1294–1309

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Modeling curvature effects in diffusion flames using a laminar flamelet model

Yuan Xuan [a,*], Guillaume Blanquart [b], Michael E. Mueller [c]

[a] Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, USA
[b] Department of Mechanical Engineering, California Institute of Technology, Pasadena, USA
[c] Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, USA

ARTICLE INFO

Article history:
Received 19 June 2013
Received in revised form 29 October 2013
Accepted 29 October 2013
Available online 20 November 2013

Keywords:
Curvature
Diffusion flames
Diffusion flamelet model

ABSTRACT

The goal of this paper is to investigate the effects of curvature of mixture fraction iso-surfaces on the transport of species in diffusion flames. A general flamelet formulation is derived mathematically considering both curvature effects and differential diffusion effects. These theoretical results suggest that curvature does not play a role in the transport process irrespective of the flame curvature if species transport is described with a unity Lewis number. On the other hand, a curvature-induced term becomes explicit when differential diffusion effects are considered, and it acts as a convective term in mixture fraction space. It is found that this term needs to be taken into account when the radius of curvature is comparable or smaller than the local flame thickness. For the proper integration of the flamelet equations, the scalar dissipation rate and curvature dependences on mixture fraction are modeled by considering two basic curved one-dimensional flame configurations. The flamelet equations accounting for curvature effects are solved with various prescribed curvature values. Results indicate that the mass fraction profiles of species with very small or large Lewis numbers are shifted significantly in mixture fraction space by the inclusion of curvature. Differential diffusion effects are enhanced by negative curvature values and suppressed by positive curvature values. In cases where flame curvature is not uniform, the curvature-induced convective term generates gradients along mixture fraction iso-surfaces, which enhance tangential diffusion effects. Budget analysis is performed on an axisymmetric laminar coflow diffusion flame to highlight the importance of the curvature-induced convective term compared to other terms in the full flamelet equation. A comparison is made between full chemistry simulation results and those obtained using planar and curved flamelet-based chemistry tabulation methods.

1. Introduction

The steady-state flamelet model [1,2] has been a popular modeling approach in simulating both laminar non-premixed flames [3,4] and turbulent non-premixed flames [5–10]. Historically, Williams was the first to rewrite, under unity Lewis number assumption, the species transport equations by separating the diffusion normal to mixture fraction iso-contours and that in tangential directions [11]. Since then, three additional simplifications have been made to make use of the flamelet formulation in turbulent reacting flow simulations: combustion processes take place in a thin layer close to the flame front, diffusion in the direction parallel to the local iso-surface of mixture fraction is negligible, and the local flame surfaces are essentially flat. Based on these assumptions, three-dimensional turbulent flames can be modeled as an ensemble of piecewise one-dimensional flame structures, termed flamelets. While this modeling framework is very powerful, it relies on several key assumptions, whose potential impacts require further analysis.

The first key assumption concerns the species Lewis numbers. In many of the previously referenced studies of turbulent reacting flows [5,7,8], unity Lewis number transport has been assumed on the basis that molecular diffusion is negligible compared to turbulent mixing. This assumption is valid for large scale mixing in the limit of sufficiently large Reynolds number, and the transition from non-unity (under laminar conditions) to unity Lewis number (under turbulent conditions) was observed for conditional means of species mass fractions in piloted turbulent methane/air jet flames as the Reynolds number was increased [12]. However, small scale scalar dynamics can still be influenced by molecular diffusion and exhibits locally non-unity Lewis number effects. The influence of non-unity Lewis number transport on turbulence-chemistry interaction has been investigated theoretically, experimentally, and

---

* Corresponding author.
E-mail address: yxuan@caltech.edu (Y. Xuan).

0010-2180/$ - see front matter © 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.combustflame.2013.10.028

numerically by previous work [12–16], and large departures from the unity Lewis number assumption have been reported in certain cases. For laminar flames, large deviations have been found in coflow non-premixed flames when comparing results obtained with unity and non-unity Lewis numbers (e.g. significantly different flame length and width) [4,17,18].

The second key assumption concerns curvature effects which have been neglected [4,17,19–21], since the combustion of interest occurred very near to the flame front. Such close proximity to the flame front (defined as the iso-surface of stoichiometric mixture fraction) allows for the flame to be modeled as flat; therefore, curvature effects could be neglected. However, many species of interest, such as Polycyclic Aromatic Hydrocarbons (PAH), tend to be located farther away from the flame, where the flame can no longer be assumed to be flat, and flame curvature effects could potentially be substantial. The impact of curvature can be further enhanced when mixture fraction iso-surfaces are highly wrinkled by turbulent motions [22]. In other words, curvature effects might be non-negligible when the product of flame curvature by the distance from the flame front is large. Unfortunately, the effects of flame curvature on flamelet modeling for both laminar and turbulent non-premixed flames still remain not well understood.

The first laminar flamelet equations were proposed by Peters [1,2] for flat flames, under unity Lewis number assumption. These equations were extended by Pitsch [19] to take into account non-unity Lewis number effects. Williams proposed a more general flamelet formulation even before Peters without making specific assumption on the flame structure [11]. However, a unity Lewis number was assumed to describe the species transport processes. More recently, Kortschik et al. [23] attempted to derive flamelet equations accounting for curvature effects. However, the predicted curvature effects did not show full agreement with the qualitative experimental observations [24]. The curvature was predicted to still have effects on species with Lewis number close to unity, but those species were observed to be hardly affected in the experiments. In summery, no mathematical framework is able to describe the combined effects of flame curvature and non-unity Lewis number using the flamelet formulation.

The objectives of this paper are threefold:

(1) derive a consistent mathematical formulation of the one-dimensional curved flamelet with differential diffusion;
(2) model the scalar dissipation rate and curvature dependences on mixture fraction for proper integration in the curved flamelet equations;
(3) investigate the effects of flame curvature and non-unity Lewis numbers in a multidimensional configuration.

The current work focuses on laminar flames, but the same results would be applicable to low Reynolds number flames in which differential diffusion effects are potentially important. The paper is organized as follows. A new flamelet formulation including curvature effects is derived in Section 2 using a general coordinate transformation. In Section 3, two basic configurations that represent curved flamelets in turbulent combustion are studied to investigate the functional dependence of scalar dissipation rate and curvature on mixture fraction. The proposed flamelet equations are solved at various curvature values, and the results are compared to those of a planar flamelet under the same conditions. In Section 4, the importance of curvature is highlighted, and its effects are investigated based on the full chemistry simulation results for a laminar coflow diffusion flame. Finally, a summary of curvature effects under various configurations is provided in Section 5.

2. Derivation of the flamelet equations with curvature

In this section, the full flamelet equations are re-derived using a general coordinate transformation to better identify the curvature and tangential terms.

2.1. Conventional flamelet equations

For two-feed non-premixed combustion systems (e.g. fuel and oxidizer) [25], the flame structures are generally described by means of a passive scalar Z. This variable is referred to as mixture fraction and ranges from 0 to 1, corresponding to pure oxidizer and pure fuel, respectively. The evolution of this variable is governed by the following transport equation for a conserved scalar

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

where ρ is the density, $\mathbf{u}$ is the velocity, and D is the mass diffusivity for Z. This diffusivity is set to the thermal diffusivity, α. Therefore, the Lewis number for Z

$$Le_Z = \frac{\alpha}{D} \tag{2}$$

is unity.

The conventional flamelet equations were derived originally by Peters starting from the species transport equations combined with the mixture fraction transport equation (Eq. (1)) [1,2]. The following coordinate transformation was used

$$x_1 \rightarrow Z, x_2 = Z_2, x_3 = Z_3, t = \tau, \tag{3}$$

leading to the conversion of the Cartesian coordinates (x_1, x_2, x_3) into a flame attached frame of reference (Z, Z_2, Z_3).

In the original work by Peters [2], Z_2 and Z_3 are chosen to be the same as distance functions in the x_2 and x_3 directions of the original Cartesian coordinate system. By construction, these two directions (Z_2 and Z_3) are not perpendicular to the gradient of mixture fraction (they do not need to be). Therefore, they do not lie within the surface of constant mixture fraction, as shown in the schematic representation in Peters' original work (Fig. 1 in [2]). In the limit of a thin, one-dimensional flat flame, this coordinate system is appropriate and convenient to derive the flamelet equations. However, for either a thick flame or a curved flame, a coordinate system with Z_2 and Z_3 perpendicular to Z would be more appropriate to distinguish effects due to tangential diffusion/convection and those due to flame curvature.

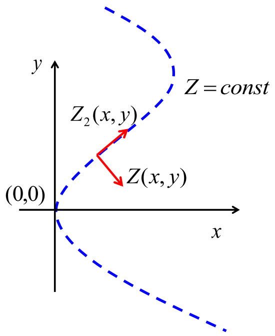

Fig. 1. Schematic of the coordinate transformation.