Combustion and Flame 163 (2016) 461–471

Contents lists available at ScienceDirect

Combustion and Flame

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

# A numerical study of laminar flames propagating in stratified mixtures

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ARTICLE INFO

*Article history:*
Received 16 May 2015
Revised 14 October 2015
Accepted 15 October 2015
Available online 13 November 2015

*Keywords:*
Stratified-charge combustion
Stratified hydrogen/air mixture
Stratified methane/air mixture
Compositional stratification
Flame speed

ABSTRACT

Numerical simulations are carried out to study flame propagation in laminar stratified fuel–air mixtures. Studies are carried out in hydrogen–air and methane–air mixtures. A 30-species 184-step skeletal mechanism is employed for methane oxidation and a 9-species 21-step mechanism for hydrogen oxidation. The study seeks to provide an improved understanding of possible differences in the local flame speed at an equivalence ratio in the compositionally stratified mixture from the speed in a homogeneous mixture at the same equivalence ratio. Flame speed and temperature profiles are evaluated and compared with corresponding values for homogeneous mixtures. As shown in prior experimental work, the numerical results suggest that when the flame propagates from a richer mixture to a leaner mixture, the flame speed is faster than the corresponding speed of the homogeneous mixture. The flame zone thickness is observed to be thinner in the stratified mixture resulting in sharper gradients. As a result, the rate of diffusion of heat and species increases resulting in increased flame speed. The effects become more pronounced in leaner mixtures. The stratification gradient influences the results with shallower gradients showing less difference in flame speeds between stratified and homogeneous mixtures. The comparative effect of thermal diffusion and species diffusion on the differences in flame speed is studied. It is shown that the species diffusion effect is more important.


## 1. Introduction

Flame propagation in compositionally stratified mixtures occurs in many applications including internal combustion engines with direct fuel injection and fires induced by leakage of fuel from storage tanks. Modeling these flames is important in improving the understanding of the physics of flame propagation and the design of the devices. For example, flame propagation speed in the combustion chamber of an internal combustion engine is one of the factors that determine the efficiency of the engine. Compositional stratification is employed in low temperature combustion engines to extend the high and low load operating limits of the engines [1–6]. Stratification also exists in direct-injection spark-ignited hydrogen and natural gas fueled engines. In these engines, direct injection is employed to extend the lean limit of operation of the engines [7–9]. Prior work suggests that flame speeds in stratified mixtures are greater than in homogeneous mixtures at the corresponding equivalence ratios. If this is the case, computational models that approximate the local flame speed at an equivalence ratio to be the flame speed in a homogeneous mixture with the same equivalence ratio would not be suitable for optimizing such engines. It is important to understand how the speed depends on the stratification. This motivates the current work.

The focus of this work is on flame propagation parallel to the compositional gradient. Kang and Kyritsis [10–12] measured flame speeds in stratified methane–air mixtures using high-speed optical visualization to observe the flame positions. A relatively rich mixture of known composition was diffused into the combustion chamber from the top of the chamber. This diffusion was opposed by a very mild counter-flow of air from the bottom of the chamber. The compositional stratification was thus achieved by the convective–diffusive balance in the chamber. The results showed that the flame propagated from the richer to leaner mixture with a faster speed than the laminar flame speed in a homogeneous mixture corresponding to the local equivalence ratio. A significant extension of the lean flammability limit was observed and explained by "back-supported" effect due to the heat diffusion from the burned gases where the temperature is higher into the leaner mixture. A similar method has been adopted to explore the propagation behavior of laminar flames into gradually richer methane/air mixture [13]. The flames are ignited in locations with close-to-stoichiometric composition. Note that the flame speed is a maximum at this composition and it decreases as equivalence ratio increases. As the flame propagates into the richer mixture, the flame is "back-supported" by heat diffusion from the region with higher flame temperature. This leads to flame speeds that are higher than the ones in homogeneous mixtures corresponding to the local equivalence ratio in the stratified mixture. Kitagawa et al. [14] investigated the flame propagation in a stratified hydrogen/air mixture. It

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http://dx.doi.org/10.1016/j.combustflame.2015.10.020
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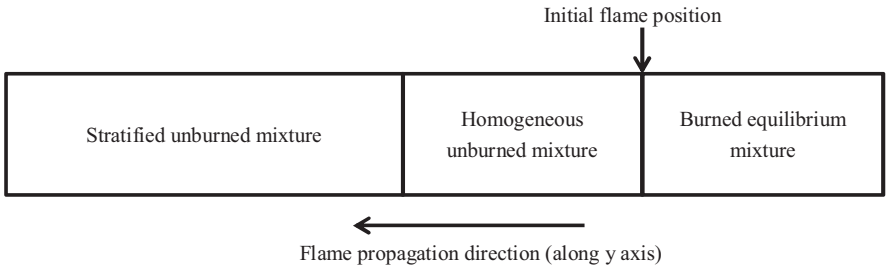


**Fig. 1.** Schematic of the computational domain.

was found that the lean flammability limit was extended by the stratification.

In addition to the experimental works cited above, Da Cruz et al. [15] have carried out numerical studies of freely propagating laminar methane/air flames in compositionally stratified mixtures. The initial configuration was that of fuel/air mixtures of different fuel concentrations with a diffusion interface at the center of the domain. The diffusion layer thickness between the two mixtures was initially a step function but grew in thickness as a result of diffusion. Results showed that the laminar flame speed was strongly affected by the equivalence ratio gradient. A change in the rate of diffusive transport of radicals and heat to the reaction zone was suggested as the key factor in explaining the behavior. All the studies cited above appear to agree on this explanation. In the current work, the compositional gradients considered are shallower than in the work of Da Cruz et al. [15] and are more representative of such gradients in engines [4]. Furthermore, the effect of Lewis number on the flame speed enhancement is studied. Lewis number is likely to be an important consideration because the explanation for the speed enhancement is based on changes in diffusive transport of heat and species.

The objective of this work is to employ direct simulations of the laminar flame propagation to understand the physics of how flame speed is related to the compositional stratification. The outline of the rest of the paper is as follows. In the next section, the numerical method and chemical kinetics mechanisms employed in this work are described. Results and discussion follow. The predicted flame speeds in stratified mixtures are compared with those in corresponding homogeneous mixtures. The comparative influence of thermal and species diffusion on "back-support" is evaluated. The paper closes with summary and conclusions.

## 2. Computational setup and chemical kinetics

The computations are carried out with the FLEDS (Flow Large-Eddy and Direct-Simulation) code. The code solves the compressible form of the Navier–Stokes equations for multicomponent gaseous mixtures with chemical reactions. The sixth-order compact finite-difference scheme of Lele [16] is employed to spatially discretize the governing equations. The resulting discretized equations are solved using the tridiagonal matrix algorithm. A fourth order Runge–Kutta scheme is employed to perform the time-integration. Boundary conditions are implemented using the Navier–Stokes characteristic boundary conditions method of Poinsot and Lele [17], which is extended to account for multicomponent transport by Anders et al. [18]. Chemical kinetic source terms are computed through an interface with CHEMKIN-like subroutines. The effective binary diffusion coefficient model for computing species diffusion, using the method of Bird et al. [19], is implemented. The code is written in FORTRAN 90 and parallelized using the message passing interface library. The code has been employed in prior studies for direct simulations of laminar flames, turbulent flames, and large-eddy simulations of jets [20–22,23].

The physical configuration studied in this work is that of an adiabatic flame propagating in a one-dimensional domain. The domain is divided two parts as shown in Fig. 1. The left part contains the compositionally stratified unburned mixture. The right part contains a homogeneous fuel/air mixture. Part of the homogeneous mixture (the part to the right of the "initial flame position") is initialized with the equilibrium temperature and composition of a burned equilibrium mixture. A linearly stratified gradient is specified in the left part. The initial species and temperature profiles in the flame are specified as follows:

$$f(y) = \left(\frac{f_U + f_B}{2}\right) + \left(\frac{f_B - f_U}{2}\right)\tanh\left(\frac{y - y_c}{\delta}\right), \quad (1)$$

where $f(y)$ is a general parameter which can represent mass fraction of species $Y_i$ or temperature $T$ as a function of $y$ location. $y_c$ represents the location where $f(y)$ is half-way between the maximum and minimum values. The parameter $\delta$ is a measure of the flame thickness. $f_B$ and $f_U$ are the burned and unburned mixture values. The hyperbolic tangent profile has been selected in many prior numerical studies of mixing layers or to mimic the profile across a flame [24–32]. After the start of the calculation, a time period is required for the flame speed to equilibrate to that of the laminar flame corresponding to the homogeneous mixture. The distance from the initial flame position to the stratified mixture is selected such that the flame can stabilize and reach its steady speed and structure before propagating into the stratified region. The pressure is 1 bar. Periodic boundary conditions are imposed on boundaries parallel to the flame propagating direction.

The resolution of the domain is dependent on the flame thickness. The flame thickness in this study varies from 0.4 mm for the hydrogen flame at 300 K, 1 bar, and equivalence ratio of 1.0–0.6 mm for the methane flame under the same conditions. The flame is thicker for lower equivalence ratios. The grid points are uniformly distributed in the domain. The effect of grid resolution on the results was assessed. Prior studies of premixed laminar flame propagation by Wang and Abraham [32] showed that 10 cells in the diffusion layer are enough to resolve the flame speed and structure when using FLEDS. In this work, up to 20 cells are employed in the flame. Figure 2 shows results of temperature, heat release rate, H mass fraction, and OH mass fraction in a premixed flame for a mixture with $\phi = 0.9$ when the grid resolution is progressively increased. It can be seen that the results with the 20 and 10 μm resolutions are about the same suggesting that 20 μm is adequate to resolve the flame. Notice that the flame thickness here is about 400 μm. The 20 μm grid size corresponds to the resolution level that there are 20 cells employed in the flame. While not shown, the flame speeds with these two finer resolutions was determined to be 1.95 m/s in both cases. The flame speeds are over-predicted when using 40 μm and 100 μm resolutions. The study was repeated for a mixture with $\phi = 0.6$ and the results are shown in Fig. 3. Once again, the results show that the grid independence is achieved with a resolution of 20 μm. These results are consistent with the earlier findings of Wang and Abraham [32].