Combustion and Flame 196 (2018) 386–399

Contents lists available at ScienceDirect

Combustion and Flame

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

Genesis and evolution of premixed flames in turbulence

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ARTICLE INFO

Article history:
Received 26 August 2017
Revised 21 October 2017
Accepted 26 June 2018

Keywords:
Turbulent premixed flames
Lagrangian methods
Backward tracking
Leading points

ABSTRACT

Flames interacting with turbulence are continuously generated and annihilated by stretching and folding processes over a range of length-scales and time-scales. In this paper, we address: from where and how do the complex topology and physico-chemical state of a fully developed turbulent premixed flame generate and evolve in time by analyzing the motion of flame particles. Flame particles are points that co-move with reactive isoscalar surfaces which are representative of turbulent premixed flames. Direct Numerical Simulation (DNS) of H_2-air turbulent premixed flame with detailed chemistry is combined with a computational methodology called the Backward Flame Particle Tracking (BFPT) algorithm. Uniform distribution of flame particles that entirely span isotherms at time t_f is tracked backwards to an earlier time t_i ($t_i < t_f$). On backtracking, the once uniformly distributed flame particles form multiple clusters in the leading locations of the corresponding isotherms. Since Zeldovich, such leading locations or leading points have remained an enigmatic concept in combustion literature inducing strong hypotheses without concrete proofs on their role. The critical observation that entire flame surface evolves from multiple clusters of leading points at earlier time allows a Finite Strain Theoretic description of the turbulent flame in terms of these points. Stretching is initiated by flame propagation along the direction of maximum curvature. Using Finite Strain Theory, we observe that at the flame surface around the leading points, the direction of minimum curvature gets preferentially aligned with the most extensive direction of the left Cauchy-Green strain-rate tensor and vorticity. These two stretching mechanisms cause the leading regions to become finite sized surfaces, several of which subsequently join together generating the complete surface at t_f. A relationship is developed between the turbulent flame speed at time t_f and the flame displacement speed and flow-flame properties like stretch-rate of the leading points from an earlier time. Finally, we have used two distinct sets of flame particles: Set-G and Set-D, which generate and destroy the flame surface, respectively. Using the observations that the flame particles in these sets follow a modified Batchelor's pair dispersion law, we have identified an important length-scale known as the Gibson scale. Curved flame propagation dominates dispersion of flame particles upto Gibson scale, while turbulence dominates dispersion of flame particles beyond this scale.

1. Introduction

Turbulence-flame interactions are present in many natural phenomena and engineering devices. Due to the nonlinear, multi-scale interactions between turbulence and the flame, the resultant flame topology is complex and average flame propagation rate is faster than the corresponding laminar flame. Understanding these complex interactions are critical for developing efficient land and aero-propulsion engines [1], preventing industrial explosions [2,3], and deciphering Supernovae Ia [4,5].

A premixed flame could be considered as an ensemble of propagating isoscalar surfaces. In several investigations, the flow-flame properties are extracted and averaged on such surfaces to investigate turbulence-flame interactions. Several of these studies assessed the statistics of alignment of the flame surface normal with the vorticity and eigenvectors of the Eulerian deformation-rate tensor S_{ij} [6–8] and/or the statistics of the constituents of the stretch-rate [9]. Eulerian analyses have also been performed to obtain statistics of several other important parameters such as flame surface area, turbulent flame speed, strain-rates, and curvature [10].

A Lagrangian approach [11–13] to investigate local dynamics of non-reacting turbulence is well known to be insightful. Parameters which are relevant to understand turbulent premixed flames have also been studied by following propagating surface elements in turbulent flows [14]. In a separate study [15], infinitesimal surface area elements were tracked in a numerically simulated homogeneous isotropic turbulent flow to assess the distributions of

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https://doi.org/10.1016/j.combustflame.2018.06.030

curvature and strain-rates. However, these surface elements were not reactive and collectively did not form a single surface, like the ones in [16]. Recently, the use of Lagrangian methods to investigate fundamental problems in turbulent combustion is gaining momentum [16–23]. The tracking methodology can be different depending on what is being tracked. While the methodology of tracking fluid particles/parcels [17–19,22,23] that shares the heritage of well-established practices from the non-reacting turbulence community has started to provide a deeper understanding, a different Lagrangian-type method which tracks particles co-moving with a flame surface has provided new insights on flame propagation and dispersion [16,20,21]. Each sub-category of the Lagrangian tracking has its own benefits and limitations when used to understand turbulence-flame interactions. While tracking fluid particles gives a material description, tracking points on a flame surface provide us with the time-history of specific portions and associated properties of the flame surface. This methodology of tracking points on a flame surface is known as the Flame Particle Tracking (FPT). It has been developed as a computational diagnostic tool based on the rigorous foundations developed by Pope [24] and offers a new paradigm for investigating turbulence-flame interactions.

In the FPT algorithm [16], spatio-temporally evolving points, called flame particles, defined on reactive isoscalar surfaces which propagate relative to the local fluid velocity are studied. A flame particle placed on an isoscalar surface is uniquely identified by $\boldsymbol{X}^F(\psi_0)$. Here, $\boldsymbol{X}$ is the initial position, ψ_0 is the isovalue of the scalar ψ, and superscript F identifies the corresponding parameter at a flame particle's position. The evolution of the position of a flame particle is governed by [16,24]:

$$\frac{\partial \boldsymbol{x}^F(\boldsymbol{X}^F(\psi_0), t)}{\partial t} = \boldsymbol{v}^F(\boldsymbol{X}^F(\psi_0), t) = \boldsymbol{u}^F + S_d^F \boldsymbol{n}^F \tag{1}$$

For brevity, the extended notation is dropped after the rightmost equality in Eq. (1). Here, $\boldsymbol{x}^F$ is the current position, $\boldsymbol{u}^F$ is the local fluid velocity, S_d^F is the local flame displacement speed relative to $\boldsymbol{u}^F$, $\boldsymbol{n}^F$ is the local surface normal pointing towards unburnt reactants, and $\boldsymbol{v}^F$ is the resultant velocity in a fixed frame of reference.

A premixed flame interacts with turbulence over multitude of length-scales and time-scales [17,25–38] causing certain regions of the flame to annihilate or extinguish, resulting in the reduction of burning area [16,20,39,40]. But, for a statistically steady configuration, the flame must be continuously generated to balance the annihilation processes. However, the locations on a flame surface that would generate the new surface are not known *a priori*. When a uniform distribution of flame particles is tracked in forward time, they cluster in the negatively curved (concave to unburned reactants) regions of the flame surface and eventually annihilate in ellipsoidal flame islands of negative curvature [20]. To circumvent this problem, the backward tracking algorithm for non-reacting fluid particles [41] is modified and complemented with the FPT algorithm. This enables tracking the flame particles backward in time, i.e., from time t_f to t_i, where $t_i < t_f$. While backtracking, the governing equations are not solved again, but the Eulerian fields saved from the DNS are read backwards, like a movie played in reverse. Backward tracking of particles in fluid flows have been found to be insightful in identifying source locations of pollutants [42] and marine organisms [43,44], fluid mixing in micro-channels [41], and to identify Lagrangian structures [13] in a turbulent flow-field. Unlike fluid particle, backtracking of flame particles has a constraint that the flame particles must always remain on their resident isoscalar surface. With the help of these backtracked flame particles, we address the following specific questions concerning turbulent premixed flames:

1. Where do the fully developed isoscalar surfaces, which are representative of a turbulent flame, evolve from? If the locations of generation of new surface are identified using flame particles, what are the special flow-flame properties that characterize these flame particles?
2. What governs the evolution of these generation locations toward a fully developed state? What could be a suitable mathematical description?
3. Could the turbulent flame speed S_T, at time t_f, be obtained as a function of the local property S_d and other flow-flame properties at these generation locations?
4. Is there any law that governs the dispersion of these flame particles? If so, could that law be used to shed light on why the flame surface must evolve from the specific locations from an earlier time?

This study is organized as follows. In Sections 2 and 3, we briefly describe the DNS databases and the BFPT algorithm. Subsequently, in Section 4, we discuss the results highlighting the role of the leading points in governing turbulent premixed flame dynamics, followed by conclusions.

2. DNS database

Two cases of DNS of H_2-air premixed flames at an equivalence ratio of $\phi = 0.81$ and at atmospheric pressure in an inflow-outflow configuration were performed using the open-source Pencil code [45]. Detailed kinetics of 9 species and 19 reactions [46] was used. The derivatives are evaluated using explicit finite difference schemes. The code uses 6th order accurate central difference scheme for spatial discretization and 3rd order accurate RK3-2N scheme for temporal discretization. In Case-1, a cuboid of size $1.918 \times 0.48 \times 0.48$cm was used. Along X, Y, and Z direction, $960 \times 240 \times 240$ grid points were used. Navier-Stokes Characteristic Boundary Condition (NSCBC) [47] along the X direction and periodic boundary condition along Y and Z directions were specified. The planar, laminar flame was initialized at some distance downstream from the inlet YZ plane. The isotropic turbulence is generated by forcing low wave-numbers in a cube containing the reactant mixture. For this cube, periodic boundary conditions on all six faces were specified. The simulation is performed till a statistically stationary state displaying Kolmogorov-Obukhov's (KO) -5/3 spectrum is reached. This isotropic turbulence at 310K, superimposed on a mean flow, is then issued from the inlet YZ plane of the cuboid. The turbulence interacts with the planar premixed flame by stretching and folding the flame at a multitude of length-scales and time-scales. In Case-1, $\Delta x/\eta \approx 1.25$. Δx is the grid spacing and $\eta = (\nu^3/\langle\epsilon\rangle)^{1/4}$ is the Kolmogorov length-scale. ν and $\langle\epsilon\rangle$ are the kinematic viscosity and mean dissipation rate in the unburnt reactants, respectively. $\delta_L/\Delta x \approx 18$. δ_L is the thermal thickness of an unperturbed, planar, laminar flame. These parameters indicate sufficient spatial resolution of the turbulence and the premixed flame, respectively. The large length-scale in unburned reactants is, $L_0 = k^{3/2}/\langle\epsilon\rangle = 0.3$cm, where k is the turbulent kinetic energy. The Taylor-scale Reynolds number, $Re_\lambda = 86$. After a fully developed turbulent flame is realized, the snapshots of the Eulerian fields are saved for 250μs, at sub-Kolmogorov time interval of $\Delta t = 1\mu s$. Kolmogorov time-scale $\tau_\eta = (\nu/\langle\epsilon\rangle)^{1/2} = 12\mu s$. Case-2, which is used for testing the generality and validity of the statistical results from Case-1, corresponds to a similar configuration but with different parameters. Details for both the cases are given in Table 1. The DNS data were then processed using the BFPT algorithm.