



Lagrangian analysis of high-speed turbulent premixed reacting flows: Thermochemical trajectories in hydrogen–air flames



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ABSTRACT

A Lagrangian analysis approach is used to examine the effects of high-speed turbulence on thermochemical trajectories in unconfined, stoichiometric hydrogen–air (H_2 –air) premixed flames. Two different intensities of turbulence in the unburnt reactants are considered, giving premixed flames with Karlovitz numbers of roughly 150 and 450. These two cases are modeled using direct numerical simulations (DNS) with both multi- and single-step H_2 –air reaction kinetics. In each of the four resulting simulations, trajectories of fluid parcels are calculated using a high-order Runge–Kutta method, and time series of temperature and chemical composition within each parcel are recorded. The resulting thermochemical trajectories are used to examine the evolution of thermodynamic quantities and chemical composition, as well as measure fluid parcel residence times and path lengths during different phases of the combustion process. Fuel mass fraction and temperature within fluid parcels are shown to be frequently non-monotonic along fluid trajectories in both single- and multi-step H_2 –air simulations, and the prevalence of non-monotonic trajectories increases with increasing turbulence intensity. Using results from single-step simulations, it is shown that this non-monotonicity can be caused solely by molecular transport processes resulting from large gradients in temperature and species concentrations created by turbulent advection. As a related consequence of advection, fluid parcel residence times are found to be smaller than in a laminar flame and the ratio of turbulent to laminar residence times decreases from roughly 0.8 to 0.6 as the turbulence intensity increases. By contrast, fluid parcel path lengths in the present high-speed turbulent flames are found to be substantially greater than laminar path lengths, resulting in fluid parcels that travel 4 and 7 times further than in a laminar flame for the two different turbulence intensities considered here.

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1. Introduction

Turbulent premixed combustion is a multi-scale, multi-physics problem involving coupled nonlinear interactions between turbulence and chemical reactions. For sufficiently high turbulence intensities, in particular, flame surfaces undergo substantial wrinkling and the internal structure of the flame, including the spatial region over which reactions occur, may become broadened relative to the structure of the corresponding laminar flame [1–4]. These changes, in turn, suggest a potentially large impact of turbulence on the evolution of thermodynamic (e.g., temperature and density)

and chemical (e.g., species mass fractions) quantities in different regions of the flame. The focus of the present study is to understand these impacts using Lagrangian analyses of high-speed turbulent premixed reacting flows.

In general, the study of turbulence effects on thermodynamic and chemical (i.e., thermochemical) quantities in premixed reacting flows is made difficult by the concurrent, coupled, and often competing effects of turbulent advection, molecular transport, and chemical reactions. The latter two effects, in particular, affect the chemical composition and temperature of fluid parcels as they are advected by the turbulent flow. The difficulty in separating each of these effects has resulted in continued uncertainty regarding predictions of flame structure for different Damköhler (Da) and Karlovitz (Ka) numbers. Furthermore, significant changes in thermochemical properties of fluid parcels in highly turbulent

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settings can have important implications for the validity and accuracy of reaction kinetics mechanisms developed and calibrated for more idealized conditions, for example those of a laminar flame or a perfectly-stirred reactor. Conditional analyses based on location within the flame have become common for the study of turbulence-chemistry interactions (e.g., [3–10]) but, even though such approaches yield valuable insights, they cannot reveal the full thermochemical evolution of a fluid parcel. These approaches also do not typically permit an unambiguous separation of advective processes from molecular transport and reactions.

In order to obtain a more fine-grained picture of turbulence-chemistry coupling in premixed reacting flows, here we employ a Lagrangian approach to track changes in chemical species concentrations and thermodynamic variables as they occur in fluid parcels during premixed hydrogen (H_2) and air combustion. We define a fluid ‘parcel’ as an infinitesimal volume whose motion is completely determined by the flow velocity, and a ‘trajectory’ is the path followed by such a parcel. A ‘thermochemical trajectory’ gives the evolution of thermodynamic and chemical properties within the fluid parcel along its path. The Lagrangian flow description is an alternative, but equivalent, representation to the more commonly used Eulerian description of fluid flows. Lagrangian analyses of turbulence have been widely used for the study of both simple and complex non-reacting flows over the last several decades, including passive scalar mixing [11], homogeneous shear flow [12], stratified homogeneous turbulence [13], and convective turbulence [14] (see also reviews by Yeung [15] and Toschi and Bodenschatz [16]). Methods and numerical algorithms for calculating Lagrangian trajectories in turbulence have also been described and discussed at length by Yeung and Pope [17] and Yu et al. [18].

Lagrangian analyses have three primary benefits in the context of premixed flame studies: (i) changes in temperature and chemical composition within a fluid parcel can be directly tracked during the combustion process, (ii) residence times and path lengths of fluid parcels during different stages of combustion (e.g., in pre-heat and reaction zones) can be computed, and (iii) effects due to molecular transport and reactions can be isolated from those due to advection. In particular, since fluid parcels exactly follow the flow and there is no advection of fluid into or out of the parcels, any changes in the thermochemical state within these parcels *must* be solely due to molecular transport and reactions. It has also been noted that flamelet-based conditional analysis approaches are poorly defined in low Lewis number thermo-diffusively unstable flames [19], providing further motivation for a Lagrangian analysis approach.

As a result of these advantages, Lagrangian analyses have become increasingly common for the study of turbulent combustion over the last several years. Steinberg et al. [20] have calculated Lagrangian trajectories from experimental measurements of a premixed dimethyl-ether and air piloted jet flame in order to examine variations in vorticity and strain rate dynamics within fluid parcels undergoing combustion. In a related study by Osborne et al. [21], it was found that residence times of fluid parcels in the flame preheat zone were almost 40% smaller, on average, than corresponding laminar flame times, despite broadening of the preheat zone by turbulence. Using a Lagrangian analysis, Day et al. have performed joint experimental and computational studies of both lean methane [19] and lean hydrogen [22] turbulent premixed flames in low swirl burners (LSB). In Ref. [22], in particular, diffusive fuel fluxes were calculated along Lagrangian trajectories, and were shown to correlate with fuel consumption rate. Despite the relatively low turbulence intensities in the LSB and similarities between turbulent and laminar trajectories, Day et al. [19,22] also noted the complex nature of thermodynamic and chemical evolutions along Lagrangian trajectories, including the non-monotonic evolution of temperature within fluid parcels. More

recently, Uranakara et al. [23] examined turbulence-induced extinction of spherical H_2 -air flame kernels using a flame particle tracking algorithm (i.e., flame surfaces, rather than fluid parcels, were tracked using a Lagrangian approach). This study showed that turbulence wrinkles flame surfaces to create “pointed” structures where increased thermal conduction leads to local and, eventually, global extinction.

The present study builds upon these prior works by specifically examining the effects of high-speed turbulence on thermochemical trajectories in premixed H_2 -air flames, where the intensity of the turbulence is characterized by the magnitude of turbulent velocity fluctuations in the unburnt reactants relative to the laminar flame speed. In such high-speed cases, turbulent advection has an increasingly dominant effect on premixed flame structure, and even greater complexity can be expected than in the studies by Day et al. [19,22]. Ultimately, our primary focus is to determine how and to what extent thermochemical trajectories vary as the turbulence intensity is increased. To this end, we seek to address the following questions: (i) How do the characteristics of thermochemical trajectories in high-speed premixed flames differ from those in laminar flames? (ii) How do these characteristics depend on turbulence intensity? (iii) What are the roles of advection, reaction, and diffusion in creating non-monotonic thermochemical trajectories? and (iv) How are fluid parcel residence times and path lengths affected by turbulence? An answer to the last question, in particular, will provide insight into the accuracy of chemical models developed for idealized conditions such as those of a laminar flame or a perfectly stirred reactor.

In order to address these questions, we examine data from direct numerical simulations (DNS) of stoichiometric H_2 -air premixed flames at atmospheric conditions. Chemical kinetics are modeled using both multi- and single-step mechanisms, and large scale turbulence velocities considered are 16 and 32 times greater than the corresponding laminar flame speeds. The turbulence in these reacting flows is thus high-speed, and both flames correspond to the thin reaction zones regime of premixed combustion [1].

In the following, we provide details on the numerical simulations performed, followed by a description of the Lagrangian analysis. We then outline properties of thermochemical trajectories in H_2 -air premixed flames for both multi- and single-step simulations and provide a summary and conclusions at the end.

2. Numerical simulations

The present DNS of stoichiometric H_2 -air premixed turbulent flames is performed using the code Athena-RFX [2,24,25], which uses a fully unsplit corner transport upwind scheme with piecewise parabolic spatial reconstruction and an HLLC Riemann solver [26] to solve the fully compressible, reactive-flow Navier–Stokes equations. In the simulations, both multi- and single-step models are employed for the stoichiometric H_2 -air reaction kinetics.

The multi-step reaction kinetics for H_2 -air combustion are based on the 2014 San Diego mechanism [27], which includes 21 different reactions involving 8 reacting species: H, H_2 , O, O_2 , OH, H_2O , HO_2 , H_2O_2 , and the inert N_2 . The equation of state is that of an ideal gas with various thermodynamic functions of pure chemical species computed using the NASA seven-coefficient format [28]. Molecular transport coefficients are calculated using mixture averaging. In particular, mixture-averaged conduction as well as diffusion coefficients for each species are computed as in the TRANSPORT library [29]. Viscosity coefficients are computed using the averaging formula of order six recommended by Ern and Giovangigli [30]. Pure species shear and bulk viscosities and binary diffusion coefficients are evaluated from standard kinetic theory expressions [31]. Thermal conduction coefficients of pure species

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