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Proceedings of the Combustion Institute 36 (2017) 1793–1800

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

On the extinction of igniting kernels in near-isotropic turbulence

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Received 4 December 2015; accepted 21 September 2016
Available online 6 October 2016

Abstract

Extinction dynamics of ignition kernels of rich H_2-air mixture ($\phi = 4$, $Le > 1$) in near-isotropic turbulence, are studied using three sets of direct numerical simulations and the recently introduced *flame particle tracking*. Turbulence is found to extinguish a freshly ignited, initially spherical premixed flame kernel, which otherwise sustains in a quiescent flow field by propagating beyond the *minimum radius*. The mechanism of kernel extinction is investigated by tracking lifetime trajectories of flame particles on an O_2 mass fraction isosurface in the flame speed-curvature (S_d, κ) space using the well-known concept of minimum radius from laminar flames. The classical S-curve in the temperature-Damköhler number (T, Da) space is also analyzed. Ensemble averaged $S_d - \kappa$ and S-curves display corresponding turning points which help to elucidate the intricate mechanisms involved in turbulent premixed flame extinction dynamics. Turbulence locally wrinkles the isosurface into positively curved structures which lead to turning points in (S_d, κ) space, such that the minimum radius is never reached, locally and as an ensemble. A budget analysis of the principal curvature evolution equation highlights the role of turbulence in *bending* the surface to form positively curved, pointed structures where heat loss is enhanced, further lowering Da towards extinction.

Keywords: Direct numerical simulations; Premixed flames; Extinction; Minimum radius; Flame particle tracking

1. Introduction

The primary objective of Direct Numerical Simulations (DNS) is to gain insights into fundamental processes occurring within a turbulent flame, and develop modeling strategies [1]. In this context, the most investigated premixed combustion configurations are, (1) an initially planar flame propagating into turbulent reactants [2–11], and (2) a spherical flame kernel developed from a central ignition source and propagating into turbulent reactants outside the kernel [12–17]. These studies have yielded an understanding of the effects of turbulence on the propagation of premixed flames, in terms of variation of flame displacement speed on

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http://dx.doi.org/10.1016/j.proci.2016.09.023
1540-7489

the strain rate, local curvature etc. Currently, the DNS codes and computing practices are rather well advanced to produce high-resolution data of flow-field variables in such generic flows. However, further work remains to develop appropriate methods for interpreting these data and use them so as to gain a deeper understanding of the reacting flows [18]. Expanding ignition kernels in turbulence occur in many practical devices, such as during ignition of the fuel-air mixture in Spark Ignition (SI) engine, Stratified Charge Compression Ignition (SCCI)/Reactivity Controlled Compression Ignition (RCCI) engine, ignition-phase in a Lean Premixed Prevaporized (LPP) gas-turbine combustor, and natural phenomena like supernova-Ia explosions. Therefore, it is imperative to understand the ignition, propagation, and extinction characteristics of a freshly ignited kernel in turbulence for improved designs of the practical devices and to explain naturally occurring combustion processes.

Premixed kernel ignition study was pioneered by LeFebvre [19,20] to demarcate regions of successful ignition or otherwise for a variety of parameters such as fuel type, turbulence, and mixture ratio. In recent times, a substantial interest [21–23] has been seen to understand the effects of initial kernel radius, and of turbulence, on self-sustained combustion of ignition kernels employing single-step chemistry, whereas detailed chemical modeling is crucial to understand any dynamics involving ignition/extinction. In a different context, Pera et al. [24] studied the 2d- and 3d- kernel propagation in early stages including a semi-detailed chemistry for iso-octane ignition. In the present work, we performed 3d, DNSs including the detailed chemistry of H_2-O_2 system. Our interest is not so much in the initial radius for successful ignition as studied previously[21–23]. Rather, we focus on the possible mechanisms that prevent a hotspot from growing into a flame front in a turbulent premixture, which otherwise would successfully progress into a propagating flame in the absence of turbulence. First, we establish a condition wherein a premixed kernel just about successfully ignites in the absence of any turbulence; next we examine the effects of introducing an initial turbulence. We find that in two such simulations under different turbulence intensity levels, the mixture fails to ignite, and using the DNS data, we seek to understand the reasons for such a behavior.

2. Computations

2.1. Direct numerical simulations

Three-dimensional, reacting flow, direct numerical simulations (DNSs) are performed using the PENCIL code [25,26]. This code solves the reacting flow equations in the compressible form. In the present study, the computational domain is a cube, as shown in Fig. 1. The outflow, NSCBC boundary conditions are imposed on all the boundaries [27,28] padded with buffer zones. The thickness of the buffer zone is chosen as 10% the domain size. The detailed H_2-air mechanism consisting of 9 species and 19 reactions developed by Li et al. [29] is used to model the chemistry. Transport properties are modeled using the mixture-averaged formulation.

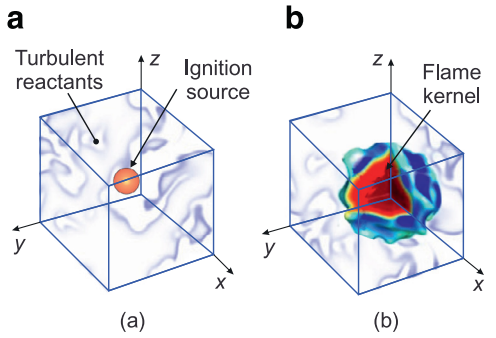

Fig. 1. Schematic of the computational domain. (a) $t = 0$, when fuel air mixture is ignited with a Gaussian profile of temperature, (b) $t > 0$, when the kernel has ignited.

Table 1
List of simulation parameters. For all cases, $T_0 = 310$ K, $p_{in} = 1$ atm, $\phi = 4$, $\mathrm{Le}_{O_2} = 2.15$, $\ell_f = 440$ μm, $\langle U \rangle = 0$ cm/s, $\nu_0 = 0.3685$ cm^2/s, and $\ell_f/\Delta_x = 21$.

	Case 1	Case 2	Case 3
Domain (cm)^3	$(0.75)^3$	$(0.5)^3$	$(1)^3$
Grid	360^3	240^3	480^3
u' (cm/s)	0	570	1095
ℓ_t (cm)	–	0.2818	0.157
τ_t (μs)	–	494	143
η (μm)	–	29.5	15.6
τ_η (μs)	–	23.6	6.6
Re_t	0	436	466
Ka_t	–	10	34
Da_t	–	2.06	0.6
$\Delta\tau_{\mathrm{track}}$ (μs)	10	2	2
τ_{track} (μs)	1010	196	190
N_{FP}	2688	1570	1510

The various parameters employed in the three DNS are listed in Table 1. Herein, Case 1 corresponds to the laminar condition ($u' = 0$) which will be used as a reference case. Cases 2 and 3 correspond to turbulent conditions. The initial velocity fields for Cases 2 and 3 are generated as non-reacting, homogeneous, isotropic turbulence (NRHIT), including all species. The fully developed NRHIT after attaining statistical stationarity is used as the initial state for the reacting flow computations. Turbulence is forced until generation of initial state but is allowed to decay in the reacting calculations. The flame kernel ignition is simulated