

Modelling of the turbulent burning velocity based on Lagrangian statistics of propagating surfaces

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We propose a predictive model of the turbulent burning velocity S_T in homogeneous isotropic turbulence (HIT) based on Lagrangian statistics of propagating surfaces. The propagating surfaces with a constant displacement speed are initially arranged on a plane, and they evolve in non-reacting HIT, behaving like the propagation of a planar premixed flame front. The universal constants in the model of S_T characterize the enhancement of area growth of premixed flames by turbulence, and they are determined by Lagrangian statistics of propagating surfaces. The flame area is then modelled by the area of the propagating surfaces at a truncation time. This truncation time signals the statistical stationary state of the evolutionary geometry of the propagating surfaces, and it is modelled by an explicit expression using limiting conditions of very weak and strong turbulence. Another parameter in the model of S_T characterizes the effect of fuel chemistry on S_T , and it is pre-determined by the very few available data points of S_T from experiments or direct numerical simulation (DNS) in weak turbulence. The proposed model is validated using three DNS series of turbulent premixed flames with various fuels. The model prediction of S_T generally agrees well with DNS in a wide range of premixed combustion regimes, and it captures the basic trends of S_T in terms of the turbulence intensity, including the linear growth in weak turbulence and the ‘bending effect’ in strong turbulence.

Key words: flames, turbulent reacting flows

1. Introduction

The turbulent burning velocity S_T measures how fast a premixed flame consumes the fresh fuel mixture in turbulence, and characterizes the impact of turbulence on the enhancement of the burning rate. The determination of S_T is one of the most important unsolved problems in turbulent premixed combustion (Peters 2000), and is critical in many models of turbulent premixed flames (Lipatnikov & Chomiak 2002; Driscoll 2008).

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In general, S_T depends on the turbulence intensity u' , flame geometry, fuel chemistry (see Lipatnikov & Chomiak 2002; Driscoll 2008) and gas expansion (Peters 2000; Sabelnikov & Lipatnikov 2017). Recent studies also investigate the dependence of S_T on the low temperature fuel chemistry (Won *et al.* 2014), high pressure (Bradley *et al.* 2013; Venkateswaran *et al.* 2014), high turbulence intensity (Wabel, Skiba & Driscoll 2017; Nivarti, Cant & Hochgreb 2019), flame stretch rates and curvatures (Thiesset *et al.* 2017).

Although there are a variety of empirical models (e.g. Bradley 1992; Lipatnikov & Chomiak 2002; Driscoll 2008) for predicting S_T and the related flame area ratio, the predictions from different models cannot collapse owing to the lack of a rigorous theoretical framework and a unique definition for S_T , and to the uncertainties of different measurement methods and flame geometries. Various power laws are used to fit data points from the experimental measurement of S_T in terms of u' , but most expressions depend on empirical parameters (e.g. Bradley 1992; Peters 1999; Lipatnikov & Chomiak 2002; Driscoll 2008; Venkateswaran *et al.* 2014; Wabel *et al.* 2017), and the corresponding scaling exponent is sensitive to flame configurations and measurements (see Verma & Lipatnikov 2016). Therefore, a consensus on the universal model for predicting S_T versus u' from experimental data remains elusive. In addition, it is possible to use the direct numerical simulation (DNS) to calculate S_T for turbulent premixed flames with a simple geometry and moderate turbulent Reynolds number Re (e.g. Tanahashi, Fujimura & Miyauchi 2000; Bell *et al.* 2005; Bell, Day & Lijewski 2013; Wang *et al.* 2017a), but the computational cost is formidable for engineering applications.

In a theoretical framework, S_T can be modelled by the Eulerian or the Lagrangian approach. Both approaches generally presume that the premixed flame is in the flamelet regime, and this assumption can be extended to the corrugated flame and thin-reaction-zone regimes with further modelling efforts (e.g. Peters 1999).

In the Eulerian approach, the local geometry and topology of the flame surface is essential to modelling methods, e.g. the flame surface density (FSD) (see Pope 1988; Candel & Poinso 1990; Trouvé & Poinso 1994; Veynante & Vervisch 2002), G-equation model (see Peters 2000), level-set methods (e.g. Creta & Matalon 2011; Yu, Bai & Lipatnikov 2015) and fractal models (e.g. Gouldin 1987; Veynante & Mebeveau 2002; Fureby 2005). In general, the flame front is extracted as the isosurface of an auxiliary scalar function, and the scalar is evolved through a partial differential equation. The additional transport equation of the Reynolds-averaged or filtered scalar field needs to be solved along with modelled conservation equations, and the modelled equations involve some empirical constants and unclosed terms which have to be modelled by further assumptions. The Eulerian modelling methods are usually used in the context of the large-eddy simulation and Reynolds-averaged Navier–Stokes simulation. Although their computational cost can be much lower than that of combustion DNS, most of them are not able or not intended to be converted to explicit expressions for S_T as the empirical correlations obtained from experiments in terms of integral quantities.

Compared with the Eulerian approach, the Lagrangian approach appears to be more natural to describe flame wrinkling with a ‘memory’ of any wrinkling occurring upstream (see Driscoll 2008; Zhou *et al.* 2019), but the Lagrangian modelling is generally restricted to non-reacting turbulence. Pope (1988) established a rigorous formulation to describe the Lagrangian evolution of surface elements in turbulent flows. To date, the Lagrangian approach has been extensively applied to investigate the local dynamics of non-reacting turbulence using material or propagating surface

elements (Girimaji & Pope 1990, 1992; Zheng, You & Yang 2017), Lagrangian particles (see Yeung 2002; Toschi & Bodenschatz 2009) and Lagrangian scalars (Yang, Pullin & Bermejo-Moreno 2010). In particular, Girimaji & Pope (1992) investigated Lagrangian statistics of the tangential strain rate and the characteristic curvature of propagating surface elements in homogeneous isotropic turbulence (HIT), which helps us to understand the deformation of premixed flames under turbulent straining motion.

Recently, the Lagrangian approach also emerged as a diagnostic tool for investigating turbulence–flame interactions in turbulent combustion. Steinberg, Coriton & Frank (2015) quantified variations of the vorticity and strain rate of fluid parcels undergoing combustion by tracking Lagrangian fluid particles and using the three-dimensional, time-resolved experimental measurement in premixed dimethyl-ether/air piloted jet flames. Day *et al.* (2015) observed the complex nature of thermodynamic and chemical evolutions along Lagrangian trajectories, including the non-monotonic evolution of temperature within fluid parcels, in a joint experimental and computational study of lean hydrogen turbulent premixed flames in low swirl burners. Hamlington *et al.* (2017) examined the effects of high-speed turbulence on the non-monotonic thermochemical trajectories in DNS of hydrogen–air premixed flames. Chaudhuri (2015) developed a method of Lagrangian flame particles to study the time history of specific portions and associated properties of the flame surface. This method has been utilized to analyse turbulence–chemistry interactions (Chaudhuri 2015) and extinction dynamics in H₂/air premixed flames (Uranakara *et al.* 2016). Dave, Mohan & Chaudhuri (2018) developed a backward flame-particle tracking method to locate the origin of the complex topology and physico-chemical state in a fully developed turbulent premixed flame.

Although the Lagrangian investigation on turbulent premixed flames serves as a valuable diagnostic tool to gain physical insights by interrogating combustion DNS data, there is a lack of predictive models of S_T from the Lagrangian perspective. Thus, we aim to incorporate the statistical information of Lagrangian surface elements into the modelling of S_T , which can bridge the gap between the studies of Lagrangian statistics in non-reacting turbulence and Lagrangian-based diagnostics in turbulent premixed combustion.

The present modelling framework of S_T is based on the Lagrangian statistics of an ensemble of propagating surface elements. The propagating surface elements, which approximate the flame surface, evolve independently via a set of ordinary differential equations for Lagrangian quantities (see Pope 1988; Girimaji & Pope 1992; Zheng *et al.* 2017). Each surface element is driven by a local fluid velocity and a displacement velocity normal to itself. The influence of molecular diffusion and chemical reaction on the motion of the flame front is only through the displacement velocity. As a simple model, the propagating surface decouples the diffusion and chemical reaction from the hydrodynamics effect on turbulent premixed combustion.

In the present study, we explore connections between S_T and the statistical geometry of propagating surfaces from a Lagrangian viewpoint, and then propose a simple predictive model of S_T in terms of u' . Most of the model parameters are pre-determined by Lagrangian statistics of propagating surfaces during a short time period in non-reacting HIT. We remark that the modelling of S_T can be very sensitive to the flame geometry, so the present flow configuration and the applicability of the proposed S_T model are restricted to HIT.

The outline of this paper is as follows. In § 2, we describe the numerical methods for the combustion DNS and tracking of propagating surfaces. In § 3, we discuss the

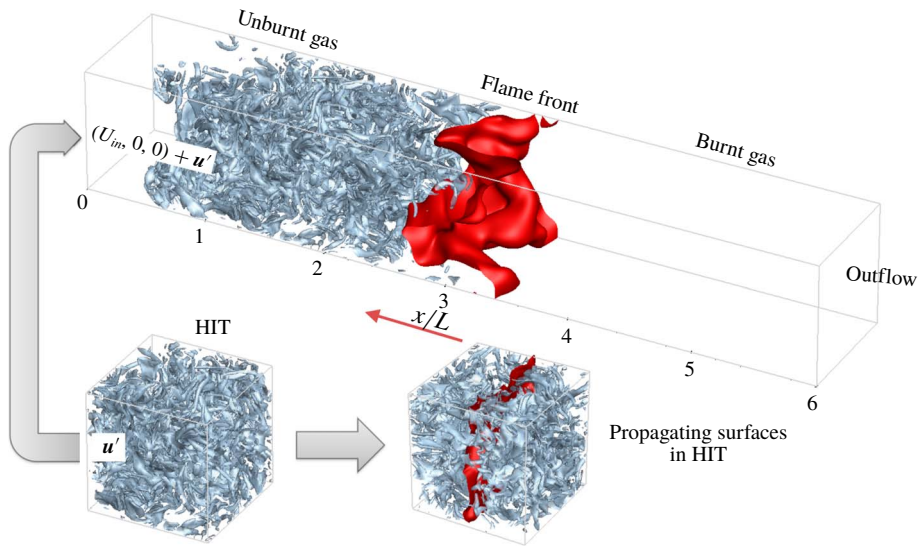


FIGURE 1. A schematic diagram of DNS configurations of the premixed flame propagation (top) and the non-reacting HIT (bottom), with light blue isosurfaces of $|\omega| = 3 \times 10^5 \text{ s}^{-1}$, the red flame front (top) and the red global propagating surface (bottom). The non-reacting HIT is utilized for the inflow condition in combustion DNS and for the tracking of propagating surfaces.

area growth of propagating surfaces, and then develop a predictive model of S_T based on the Lagrangian statistics and several physical assumptions. In §4, we present both *a posteriori* and *a priori* tests for the proposed model. Some conclusions are drawn in §5.

2. Numerical overview

2.1. Combustion DNS

For the combustion DNS, we consider the free propagation of a planar H_2/air premixed flame along the streamwise x -direction in statistically stationary HIT. This inflow–outflow DNS configuration of turbulent flames (e.g. Tanahashi *et al.* 2000; Aspden, Day & Bell 2011; Savard, Bobbitt & Blanquart 2015; Nivarti & Cant 2017; Minamoto, Yenerdag & Tanahashi 2018) is presented in figure 1. The computational domain is a cuboid with sides $L_x \times L_y \times L_z = 6L \times L \times L$ and $L = 2 \text{ mm}$. It has inflow and outflow conditions at the left and right boundaries, respectively, and periodic boundary conditions in the lateral y - and z -directions. This domain is discretized on uniform grid points $N_x \times N_y \times N_z = 6N \times N \times N$ with the mesh spacing Δx .

The unburnt gas is a lean H_2/air mixture with the equivalence ratio $\phi = 0.6$ at the temperature $T_u = 300 \text{ K}$ and atmospheric pressure. It is ignited by a planar laminar flame initially located in the middle of the computational domain. The one-dimensional steady laminar premixed flame is computed using the PREMIX code (Kee *et al.* 1985) with the nine-species detailed kinetic mechanism and mixture-averaged transport properties. The laminar flame speed is $S_L = 0.723 \text{ m s}^{-1}$, the flame thermal thickness $\delta_L \equiv (T_b - T_u)/|\nabla T|_{\max} = 0.361 \text{ mm}$ and the flame time scale $\tau_f \equiv \delta_L/S_L = 0.499 \text{ ms}$, where T_u and T_b are temperatures in the unburnt and

Case	A	B	C	D	E
N	128	128	128	256	256
u'/S_L	1.0	2.0	5.0	10.0	20.0
l_t/δ_L	0.91	0.91	0.91	0.91	0.91
T_e (μs)	1100	426	156	72.7	38.3
τ_η (μs)	144	47.6	11.9	4.21	1.53
η (μm)	52.9	30.4	15.2	9.04	5.45
$\eta/\Delta x$	3.39	1.95	0.97	1.16	0.70
Re	14.24	28.48	71.2	142.4	284.8
Ka	1.04	2.94	11.64	32.91	93.08
Da	0.92	0.46	0.18	0.09	0.05

TABLE 1. Parameters for DNS cases.

burnt mixtures, respectively, and $|\nabla T|_{\max}$ denotes the maximum temperature gradient in the laminar premixed flame.

We carried out five DNS cases with varied turbulent intensity u' listed in table 1. For the inflow condition, we first performed a separate DNS of non-reacting, statistically stationary HIT. These HIT data are then imposed on the bulk inflow velocity $U_{in}(t)$ by using Taylor's hypothesis. Thus the inflow condition is $\mathbf{u}_{in}(y, z, t) = U_{in}(t) + \mathbf{u}'(y, z, t)$ with the fluctuating velocity $\mathbf{u}'(y, z, t)$ on the y - z plane moving through the HIT field at $U_{in}(t)$. A feedback control algorithm (Bell *et al.* 2006) is applied to dynamically adjust $U_{in}(t)$ to stabilize the turbulent flame in the middle of the computational domain. The convective condition (Desjardins *et al.* 2008) is used for the velocity and scalars at the outflow boundary in the streamwise direction. A stable, linear velocity forcing (Carroll & Blanquart 2013; Savard *et al.* 2015) is adopted to maintain the turbulent intensity from $x = 0.5L$ to $5L$ along the streamwise direction in combustion DNS and in the entire domain in non-reacting DNS.

The integral length scale l , the eddy turnover time T_e , the Kolmogorov time scale τ_η and length scale η and the turbulent Reynolds number $Re \equiv u'l/\nu$ of the HIT are summarized in table 1. The Karlovitz number $Ka \equiv (u'/S_L)^{3/2}(\delta_L/l)^{1/2}$ and the Damköhler number $Da \equiv (S_L/u')(l_t/\delta_L)$ are computed in the unburnt side. In terms of the regime diagram (Peters 2000) in figure 2, case A is very close to the regime of wrinkled flamelets and laminar flames, cases B, C and D are in the thin reaction zone and case E is close to the broken reaction zone. We remark that the boundaries dividing different regimes in the Borghi diagram in figure 2 are solely based on phenomenological arguments and dimensional analysis. Thus the applicability of the diagram is still under debate for accurately characterizing flame structures (e.g. Aspden *et al.* 2011; Tamadonfar & Gülder 2015; Aspden *et al.* 2017; Wabel *et al.* 2017; Skiba *et al.* 2018), and the diagram is only presented for roughly comparing flow and flame parameters in different DNS series.

The numerical resolution in all the cases is ensured to resolve the smallest turbulent scales by the criterion $\eta/\Delta x > 0.5$ (see Pope 2000) and to resolve the flame length scales using a minimum of 24 grid points within δ_L . In addition, our grid convergence study (see supplementary material available at <https://doi.org/10.1017/jfm.2019.1081>) further validates that the present combustion DNS is sufficiently well resolved by comparing S_T and flame structures from simulations on the present grid and a coarser one.

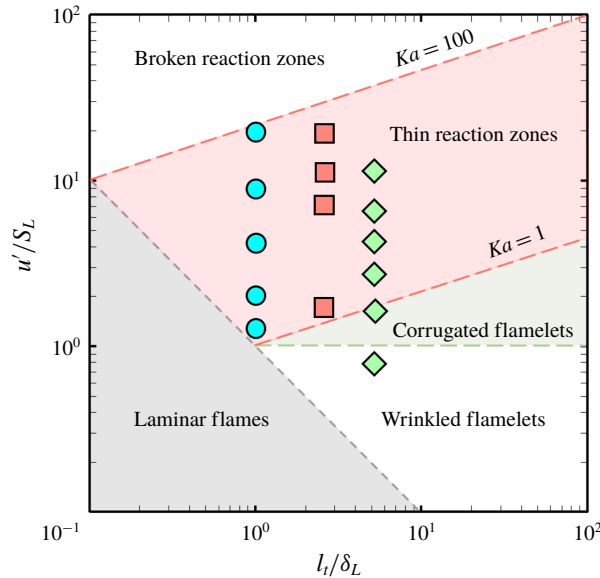


FIGURE 2. Parameters of three DNS series in the regime diagram of turbulent premixed combustion. Circles: the present DNS; squares: DNS of Nivarti & Cant (2017); diamonds: DNS (group T) of Lee & Huh (2010).

Species	H ₂	O ₂	H ₂ O	H ₂ O ₂	HO ₂	OH	H	O	N ₂
<i>Le</i>	0.27	1.04	0.79	1.03	1.04	0.67	0.16	0.66	1.01

TABLE 2. Constant species Lewis numbers.

The low-Mach-number, variable-density formulation of conservation equations of mass, momentum, species and energy are solved on staggered grid points using the NGA code (Desjardins *et al.* 2008). A second-order centred, kinetic-energy conservative finite difference scheme is used to discretize the spatial derivatives in the momentum equations. A third-order bounded QUICK scheme (Herrmann, Blanquart & Raman 2006) with low numerical dissipation and preserved physical bounds of scalars is adopted to treat convection terms in the scalar transport equations of species mass fractions and temperature, and this scheme has been used in a series of DNS of turbulent premixed flames (e.g. Savard *et al.* 2015; Bobbitt, Lapointe & Blanquart 2016). The temporal integration of the conservation equations is advanced by an iterative semi-implicit Crank–Nicolson scheme (Pierce 2001). The detailed nine-species H₂/air kinetic mechanism is employed with reaction rates, thermodynamic properties are evaluated by the CHEMKIN (Kee *et al.* 1996) library. The constant Lewis numbers listed in table 2 are used in DNS and they are determined from the fit in terms of mixture-averaged transport properties for the laminar premixed flame. The time integration of chemical source terms is performed using the stiff DVODE solver (Brown, Byrne & Hindmarsh 1989). Each DNS case is first run for at least $10T_e$ to reach a statistically stationary state, and then statistical properties of interest are calculated over a period of $20T_e$.

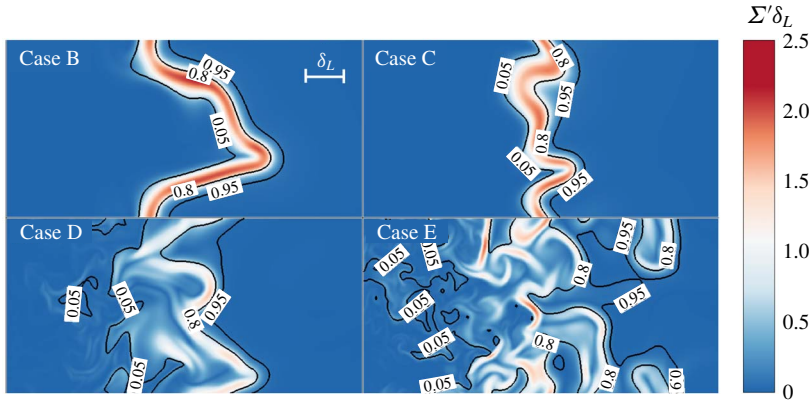


FIGURE 3. Normalized local FSD $\Sigma'\delta_L$ on a slice of size $2L \times L$ centred at $x = 3L$ and at $t = 20T_e$ from four combustion DNS cases.

We define a reaction progress variable

$$c \equiv \frac{Y_f - Y_{f,u}}{Y_{f,b} - Y_{f,u}} \quad (2.1)$$

to characterize the progress of reaction and flame propagation, where Y_f is the fuel mass fraction, $Y_{f,u}$ and $Y_{f,b}$ are the fuel mass fractions in unburnt and burnt mixtures, respectively. The isosurface of $c = \hat{c}$ propagates at a displacement speed S_d . The instantaneous flame front is chosen such that $\hat{c} = 0.8$ corresponds to the location of the maximum heat release rate in the unstrained laminar flame.

Figure 3 depicts contours of the normalized local FSD $\Sigma'\delta_L$ on a slice near the flame front at $t = 20T_e$ in combustion DNS cases B, C, D and E, with three isolines of $c = 0.05, 0.8$ and 0.95 to characterize the turbulent flame brush. Here, the large local FSD generally characterizes the flame front, and the detailed definition of the FSD is explained in appendix A. The laminar flamelet structure is retained in most of the flame brush in case B, and the flamelet structure in the preheat zone is disturbed and progressively broadened in cases C and D. The topology of the reaction layer, as the isosurface of $c = 0.8$, still retains sheet-like parallel surfaces in both cases in the thin reaction zone. With increasing Ka , some portions of the flame front are broken down in case E.

2.2. Tracking of propagating surface elements

As sketched in figure 1, the non-reacting HIT field used in the inflow condition of combustion DNS is also utilized in the tracking of propagating surface elements. For each DNS case listed in table 1, an ensemble of infinitesimal propagating surface elements are initially arranged on a planar surface in non-reacting HIT to model the propagation of a turbulent premixed flame.

Each propagating surface element carries the information of its Lagrangian location $\mathbf{X}(t)$, local coordinate system $\mathbf{e}_i(\mathbf{X}(t), t)$, curvature tensor $h_{\alpha\beta}$ and nominal surface area δA (Pope 1988). The evolution equation of $\mathbf{X}(t)$ is

$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{u}(\mathbf{X}(t), t) + S_d(\mathbf{X}(t), t)\mathbf{n}(\mathbf{X}(t), t). \quad (2.2)$$

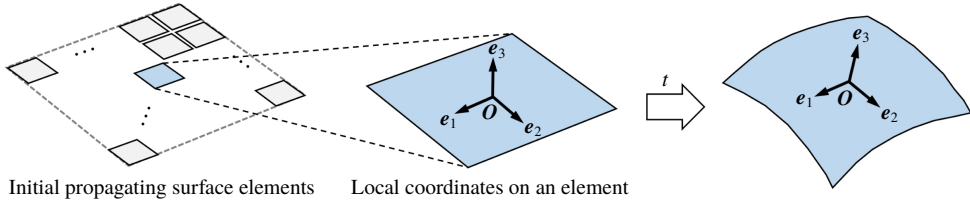


FIGURE 4. Sketch of the temporal evolution of the propagating surface elements.

Each surface element moves with the local fluid velocity \mathbf{u} and the displacement velocity $S_d \mathbf{n}$, where \mathbf{n} denotes the unit normal of the surface element, and the displacement speed S_d can be simply modelled by a constant S_L or a variable accounting for the effect of weak flame stretch.

As sketched in figure 4, a local Cartesian coordinate system $\mathbf{e}_i(\mathbf{X}(t), t)$, $i = 1, 2, 3$ is attached to each surface element in order to compute \mathbf{n} and other geometric properties of the surface elements. Its origin, denoted by ‘O’, is at the position $\mathbf{X}(t)$ of the surface element. The unit normal vector \mathbf{e}_3 is equivalent to \mathbf{n} in (2.2), and two orthogonal unit vectors \mathbf{e}_1 and \mathbf{e}_2 span the tangent plane.

The governing equations for this coordinate system are

$$\left. \begin{aligned} \frac{d\mathbf{e}_3}{dt} &= -\mathbf{e}_\alpha u_{3,\alpha}, \\ \frac{d\mathbf{e}_\alpha}{dt} &= \frac{1}{2} \mathbf{e}_\beta (u_{\beta,\alpha} - u_{\alpha,\beta}) + \mathbf{e}_3 u_{3,\alpha}, \quad \alpha, \beta = 1, 2, \end{aligned} \right\} \quad (2.3)$$

where ‘ α ’ denotes the partial derivative in the direction of \mathbf{e}_α . The governing equation of the curvature tensor $h_{\alpha\beta}$ is

$$\frac{dh_{\alpha\beta}}{dt} = s_{33} h_{\alpha\beta} - (s_{\gamma\beta} h_{\alpha\gamma} + s_{\gamma\alpha} h_{\beta\gamma}) + u_{3,\alpha\beta} + S_d h_{\alpha\gamma} h_{\gamma\beta}, \quad (2.4)$$

where the partial derivatives of S_d are neglected (Zheng *et al.* 2017) and

$$s_{ij} \equiv \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad i, j = 1, 2, 3 \quad (2.5)$$

denotes the local rate-of-strain tensor. Principal curvatures κ_i , $i = 1, 2$ of a surface element are defined as $\kappa_i = -k_i$ with $\kappa_1 > \kappa_2$, where k_i , $i = 1, 2$ are eigenvalues of $h_{\alpha\beta}$. A surface element convex (or concave) to the propagating direction \mathbf{n} has a positive (or negative) curvature.

At time t , $\delta A(t)$ denotes the nominal surface area, which can also be considered as the area ratio of infinitesimal surface elements. The governing equation of $\delta A(t)$ or the surface stretch rate K of the propagating surface is

$$K \equiv \frac{1}{\delta A(t)} \frac{d\delta A(t)}{dt} = K_t + 2S_d \kappa, \quad (2.6)$$

where the tangential strain rate $K_t \equiv u_{1,1} + u_{2,2}$ characterizes the stretching of the surface area due to the straining by the flow field, and $2S_d \kappa$ with the mean curvature $\kappa \equiv (\kappa_1 + \kappa_2)/2$ represents the fractional rate of change of area due to propagation.

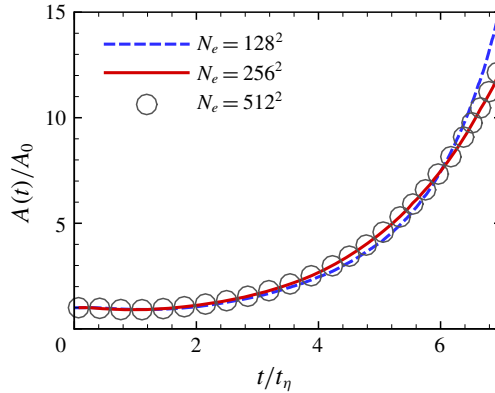


FIGURE 5. Convergence test of the number of propagating surface elements in non-reacting DNS case C.

At the initial time, $N_e = 256^2$ surface elements are uniformly arranged on an x - y plane at $z = L/2$ to model a propagating planar flame in premixed combustion (see figures 1 and 4). Each surface element has $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) = (0, 0, 1)$, $h_{\alpha\beta} = 0$ and $\delta A(0) = A_0/N_e$, where $A_0 \equiv \sum_{N_e} \delta A(0)$ is the initial global surface area. A convergence test with increasing N_e in figure 5 shows that the total surface area ratio, which is defined later in § 3.2, from $N_e = 256^2$ surface elements is almost identical to that from $N_e = 512^2$, so $N_e = 256^2$ is used in the present study. Additionally, our grid convergence study (see supplementary material) validates that the present non-reacting DNS is sufficiently well resolved to calculate Lagrangian statistics of propagating surfaces.

The tracking of propagating surface elements begins when the non-reacting HIT has reached the statistically stationary state. A second-order, symmetry-preserved Runge–Kutta scheme (Zheng *et al.* 2017) is applied to advance (2.2), (2.3) and (2.6) explicitly and (2.4) implicitly. The time increment is sufficiently small to resolve the finest scales of the velocity field. The Fourier spectral method is used to evaluate the velocity derivatives involved in these equations. The interpolation is performed by a sixth-order Lagrangian interpolation scheme. In addition, the propagating surface elements can evolve into cusps after a finite time (Girimaji & Pope 1992), and these cusps are removed in the tracking based on the positive definiteness of the curvature tensor. The detailed numerical implementation of the surface tracking and the criterion for detecting cusps are described in Zheng *et al.* (2017), and numerical errors have been verified to be negligible. It is noted that the computational cost of the tracking of propagating surfaces in non-reacting DNS is very low, of $O(1)$ CPU hours on a single core. By contrast, the computational cost of each combustion DNS on a parallel machine is $O(10^4) \sim O(10^5)$ CPU hours.

The evolution of global propagating surfaces consisting of surface elements in stationary HIT is shown in figure 6 for cases B and D. From an initial plane, the propagating surface is gradually wrinkled and corrugated by turbulent straining motion to form the cellular geometry. Compared with the persistent stretch of a passive material surface with $S_d = 0$, the evolution of a propagating surface with finite S_d can generate cusps, and cusp locations are marked by red dots. Most of the cusps are generated around the crest of the surface with large negative curvatures. This ‘pocket structure’ is critical for predicting the flame stabilization and pollution formation in turbulent premixed combustion (Bell *et al.* 2013). At the same normalized time

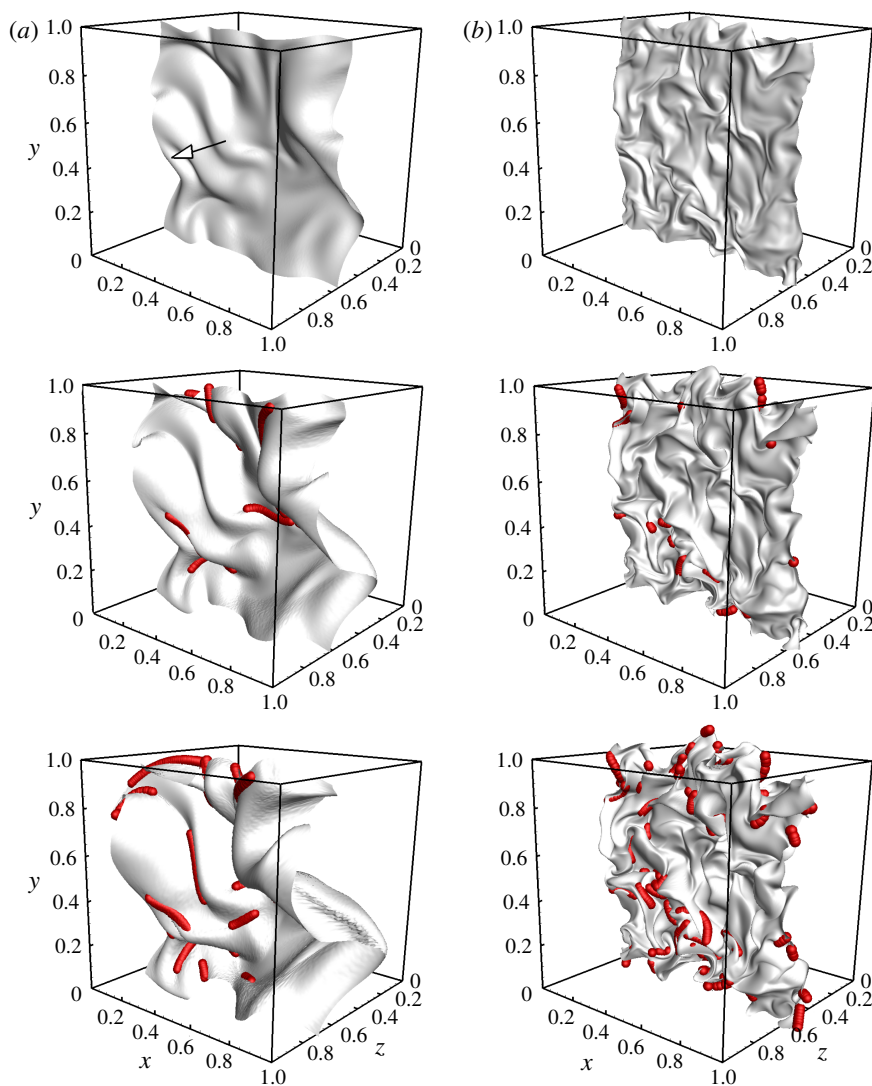


FIGURE 6. Temporal evolution of the global propagating surface in cases B and D at $t^* = 1, 2$ and 3 (from top to bottom) in non-reacting HIT. The arrow denotes the propagation direction, and the red dots mark locations of cusp generation.

$t^* \equiv t/\tau_\eta$, the surface is more wrinkled in case D with larger turbulence intensity than in case B.

We remark that the ensemble of surface elements can only approximate the global propagating surface rather than exactly represent the real flame surface. The surface elements can be considered as sample points scattered on the global propagating surface. Moreover, the heat release in combustion can induce fluid thermal expansion and acceleration (Peters 2000; Sabelnikov & Lipatnikov 2017). The relevant density change and pressure effects can influence the turbulent flame morphology and dynamics, such as cusp formation and collision events (Fogla, Creta & Matalon 2015), and they can be coupled with the Darrieus–Landau instability

under weak turbulence (Creta & Matalon 2011; Troiani, Creta & Matalon 2015). These variable-density effects are not considered in the present non-reacting HIT, and they can be incorporated via a modelled variable-density flow in future work.

3. Model development

3.1. Turbulent burning velocity

The turbulent burning velocity is defined using the global consumption speed of fuel

$$S_T \equiv \frac{1}{\rho_u Y_{f,u} L_y L_z} \int_{\Omega} -\rho \dot{\omega}_f(x, y, z, t) d\Omega, \quad (3.1)$$

where ρ_u denotes the density of the unburnt mixture, $\dot{\omega}_f$ the net reaction rate of fuel and Ω the entire computational domain. Although there is no consensus on the best definition of S_T (Driscoll 2008), i.e. S_T can be defined by the local consumption speed or the local displacement speed, we use the global consumption speed (3.1) without the subjective selection of the isocontour threshold.

Damköhler (1940) conjectured that turbulence can enhance S_T primarily through increasing the flame surface area under a low turbulence intensity, so the ratio of the flame surface area A_T in turbulence and its projection in the propagating direction A_0 is generally equal to the ratio S_T/S_L . Thus the modelling of A_T is essential to estimate S_T under the assumption (see Driscoll 2008)

$$\frac{S_T}{S_L} = I_0 \frac{A_T}{A_0} \approx \frac{A_T}{A_0}, \quad (3.2)$$

where the stretch factor I_0 depends on the effect of differential diffusion and is assumed to be unity from the present combustion DNS results (not shown). Some other DNS studies of turbulent premixed flames in HIT with moderate and high u' (see Bell, Day & Grcar 2002; Hawkes & Chen 2006; Nivarti & Cant 2017; Wang, Magi & Abraham 2017) also observe that S_T/S_L is proportional to A_T/A_0 with nearly unity I_0 , which supports the validity of Damköhler's hypothesis for the flame propagation in HIT. It is noted that, in some jet flames under very strong turbulence (e.g. Wabel *et al.* 2017), Nivarti *et al.* (2019) argued that small-scale turbulence can serve as an effective turbulent diffusivity to enhance S_T , and this additional factor should be incorporated into (3.2).

3.2. Area growth of propagating surfaces

We model the ratio A_T/A_0 of flame surface areas by the ratio of global propagating surface areas in the DNS of non-reacting HIT. In the evolution of a global propagating surface initially consisting of N_e surface elements, only $N_s(t)$ surface elements survive. As sketched in figure 7, the other $N_d(t)$ surface elements disappear, because they evolve into cusps at a finite time and their surface areas shrink to zero (Girimaji & Pope 1992). Since these cusps cannot exist owing to smoothing effects of diffusion and curvature in real flames, these extreme samples are removed in the tracking of propagating elements (see Zheng *et al.* 2017). This removal of the cusps can be viewed as a mechanism of area reduction, and other flame destruction mechanisms, such as mutual annihilation and quenching, are implicitly involved in further modelling.

The surviving ratio $R_s \equiv N_s(t)/N_e$ of surface elements is shown in figure 8. We observe that the cusp generation occurs around $t^* = 2$ and the cusps are generated

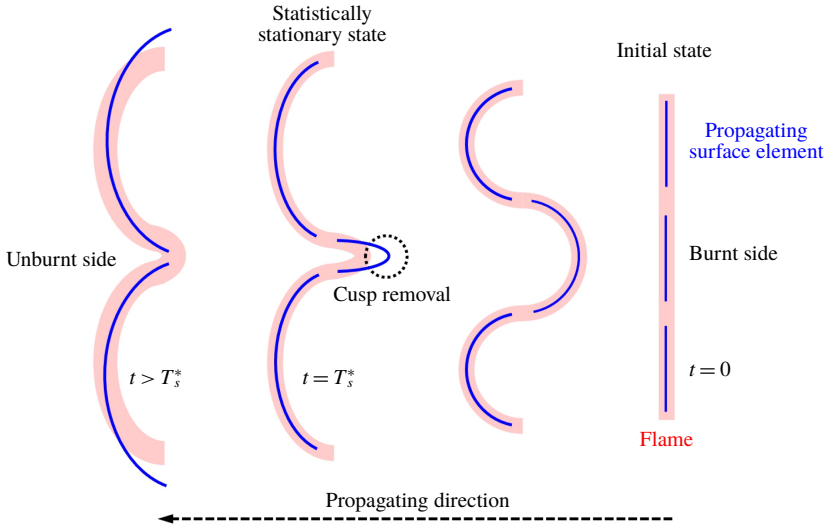


FIGURE 7. A schematic diagram of the evolution of propagating surface elements (thin blue lines) and a flame front (thick red lines).

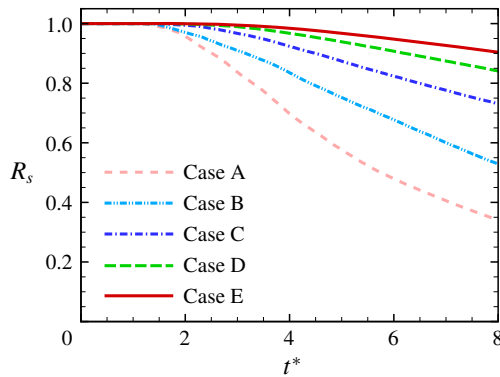


FIGURE 8. Surviving ratios of propagating surface elements in non-reacting DNS cases.

more quickly at smaller turbulence intensity. At smaller u'/S_L , the propagation term in (2.4) can dominate (see Zheng *et al.* 2017), so a surface element with a large negative curvature can more easily develop a singularity in a finite time.

It is noted that all the subsequent quantities with the superscript “*” denote the ones normalized by Kolmogorov length scale η , time scale τ_η or velocity scale u_η . Zheng *et al.* (2017) demonstrated that the profiles of ensemble-averaged κ_1^* and κ_2^* of propagating surfaces in terms of S_d^* at the statistically stationary state are almost independent of Re .

After removing the cusps, the total surface area of the global propagating surface consisting of $N_s \leq N_e$ surviving surface elements is approximated as

$$A(t) \equiv \sum_{N_s(t)} \delta A(t). \tag{3.3}$$

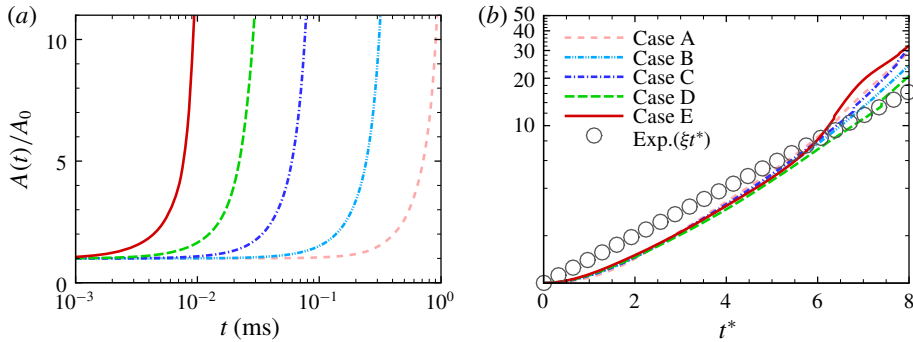


FIGURE 9. Surface area ratios of propagating surfaces in terms of (a) the physical time and (b) normalized time in non-reacting HIT.

Summing up the local quantities of $N_s(t)$ surviving surface elements in (2.6) yields the evolution equation of $A(t)$ (Zheng *et al.* 2017)

$$\frac{d}{dt} \ln A(t) = \langle K_t(t) \rangle_A + 2 \langle S_d(t) \kappa(t) \rangle_A, \quad (3.4)$$

where

$$\langle f(t) \rangle_A \equiv \frac{\sum_{N_s(t)} f(t) \delta A(t)}{A(t)} \quad (3.5)$$

denotes the area-weighted average of a quantity $f(t)$.

Integrating the normalized (3.4) from the initial tracking time $t^* = 0$ to a given time t^* yields the surface area of the global propagating surface

$$\frac{A(t^*)}{A_0} = \exp \left(\int_0^{t^*} \langle K_t^*(s) \rangle_A ds \right) \exp \left(2 \int_0^{t^*} \langle S_d^*(s) \kappa^*(s) \rangle_A ds \right). \quad (3.6)$$

This implies that the growth of $A(t)$ of the propagating surfaces is due to the Lagrangian history of statistically positive tangential strain-rate and propagation-curvature terms in the wrinkling process of propagating surfaces in turbulence (Zheng *et al.* 2017). Subsequently, S_d is assumed to be a constant laminar burning velocity S_L as

$$\frac{A(t^*)}{A_0} = \exp \left(\int_0^{t^*} \langle K_t^*(s) \rangle_A + 2S_L^* \langle \kappa^*(s) \rangle_A ds \right). \quad (3.7)$$

This assumption is justified and the effect of flame stretch on S_d is discussed in appendix B.

As implied in (3.7), $A(t)/A_0$ grows with t in figure 9(a), and its growth rate increases with Re for the same S_L , because K_t scales as $K_t \sim 1/\tau_\eta \sim Re^{1/2}$. This result is consistent with the observation that A_T of flames increases with Re in the argument of FSD modelling in appendix A. On the other hand, if t is normalized by corresponding τ_η in each case, the profiles of $A(t^*)/A_0$ for different Re collapse in figure 9(b). Similarly, the surviving ratio for the same S_L is almost independent of Re (Zheng *et al.* 2017). These indicate that Kolmogorov scales are more appropriate than integral scales for the normalization in scale analyses, and further modelling

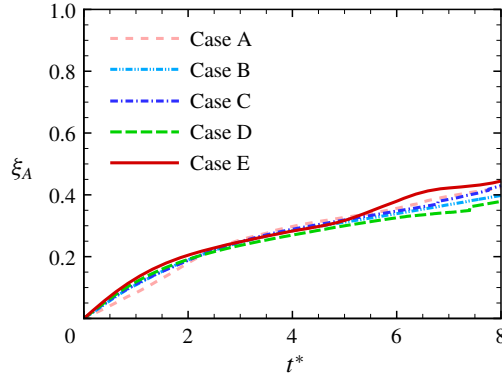


FIGURE 10. Growth rates of the surface area of propagating surfaces in non-reacting HIT.

based on the universal properties of $A(t^*)$ naturally involves the effect of Re on S_T in terms of integral quantities.

The estimation of $A(t)/A_0$ of propagating surfaces is similar to that for material surfaces in non-reacting HIT. Batchelor (1952) proposed that $A(t)/A_0$ of material surfaces grows exponentially owing to the persistent stretching of turbulent motion, which was validated by DNS (e.g. Girimaji & Pope 1990; Goto & Kida 2007; Yang *et al.* 2010). Considering the self-similar area growth of propagating surfaces at different Re , we re-express (3.7) in the form of

$$\frac{A(t^*)}{A_0} = \exp(\xi_A t^*), \tag{3.8}$$

where $\xi_A(t^*) \equiv \log(A(t^*)/A_0)/t^*$ is the area growth rate. A similar exponential growth of the flame surface was assumed by Kerstein (1988) and Yakhot (1988).

In figure 10, the area growth rates also nearly collapse, consistent with the observation in figure 9(b). For material surfaces in HIT, ξ_A approaches a statistically stationary state as $\xi_A = 0.33 \pm 0.04$ after a rapid, monotonic growth in $2 \sim 3\tau_\eta$ (see Yang *et al.* 2010). For propagating surfaces, by contrast, ξ_A does not reach the statistically stationary state, so an additional approximation is introduced to model

$$\xi_A(t^*) = \xi \tag{3.9}$$

by a constant ξ , which is addressed in § 3.5 in detail.

3.3. Introduction of the truncation time

A global propagating surface in turbulence should have $A(t) \rightarrow \infty$ as $t \rightarrow \infty$ in (3.8) owing to the persistent stretching and the lack of surface shortening mechanisms. On the other hand, the shortening mechanism in real turbulent flames may occur when adjacent flamelets consume the intervening reactant, thereby annihilating both surface elements. Thus the flame area A_T should be finite, which can be considered as a stationary random variable with competing flame stretching and shortening mechanisms (Marble & Broadwell 1977).

To resolve this contradiction, we postulate that the surface area of turbulent flames can be estimated by

$$A_T = A(T_s^*) \tag{3.10}$$

at a truncation time T_s^* when the statistical geometry of the propagating surfaces just reaches a statistically stationary state (Zheng *et al.* 2017). As sketched in figure 7, this state resembles the statistical equilibrium state in combustion between the flame area growth due to turbulent straining and the area consumption due to flame self-propagation. After this state, the nominal area of independent propagating surfaces with infinitesimal thickness can still grow (see figure 9), but the area of real flames statistically converges to a finite value. In § 3.6, we will demonstrate that the ansatz of (3.10), together with modelled T_s^* , serves as the basic analytical structure leading to a physically reasonable functional form of S_T with finite A_T , so the flame shortening mechanisms can be implicitly incorporated into the truncation time. Applying (3.8) and (3.9) to (3.10), we have the model of A_T in terms of T_s^* as

$$\frac{A_T}{A_0} = \exp(\xi T_s^*). \quad (3.11)$$

Before modelling T_s^* , we first use the characteristic curvature

$$C^* \equiv \sqrt{\kappa_1^{*2} + \kappa_2^{*2}} \quad (3.12)$$

to characterize the statistical stationary state of propagating surfaces. We find that the temporal evolution of the ensemble-averaged C^* is statistically more robust than those of K_t^* and κ^* in (3.6). The latter two are found to be very sensitive to specific realizations in DNS.

The DNS of propagating surfaces demonstrates that $\langle C^* \rangle$ can reach a statistically stationary state after a short time in figure 11(a), where $\langle \cdot \rangle$ denotes the ensemble average over all the surviving surface elements, and this result is supported by the theoretical analysis in appendix C. The temporal growth rate $d\langle C^* \rangle/dt^*$ of $\langle C^* \rangle$ is also computed and shown in figure 11(b). After a rapid growth at very small times, the growth rate decays and finally approaches a statistical stationary state. We observe that the growth rates almost collapse in cases C, D and E at moderate Re , which implies that the time T_s^* to reach the statistically stationary state of $\langle C^* \rangle$ approaches a finite value as $u'/S_L \rightarrow \infty$. Furthermore, the temporal evolution of probability density functions (PDFs) of C^* in figure 12 indicates that the PDFs at different times almost collapse after reaching the statistically stationary state around $t^* > 4$.

We denote the truncation time

$$T_\infty^* = \lim_{u'/S_L \rightarrow \infty} T_s^* \quad (3.13)$$

for $u'/S_L \rightarrow \infty$ or material surfaces, which is useful in the modelling of T_s^* in § 3.4. We approximate

$$T_\infty^* = \arg \min_{t^*} \left\{ \left| \frac{d\langle C^* \rangle(t^*)}{dt^*} \right| < \varepsilon_T \right\}, \quad (3.14)$$

by T_s^* from the DNS of propagating surfaces in case E with large u'/S_L , where $\varepsilon_T = 0.1\%$ is a small threshold. We determine $T_\infty^* = 5.5$ using (3.14) and it appears to be a universal constant, because the normalized time t^* when $\langle C^* \rangle$ of the material surfaces reaches the stationary state (Girimaji & Pope 1990; Girimaji 1991) can be almost independent of large Re owing to the self-similar statistical geometry.

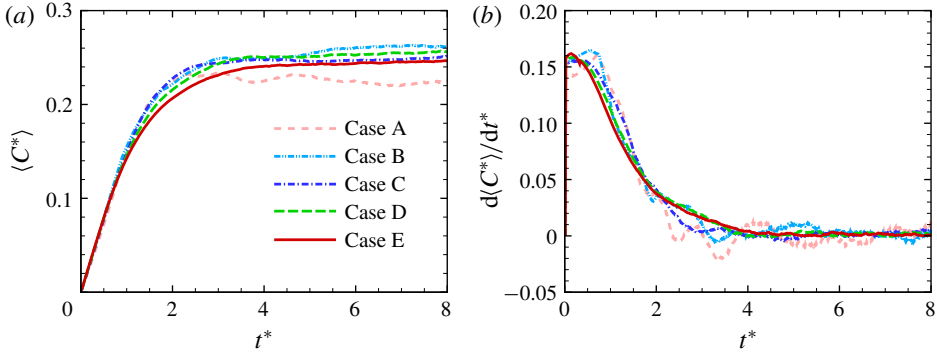


FIGURE 11. The temporal evolution of (a) the ensemble-averaged characteristic curvature and (b) its temporal growth rate of propagating surface elements in non-reacting HIT.

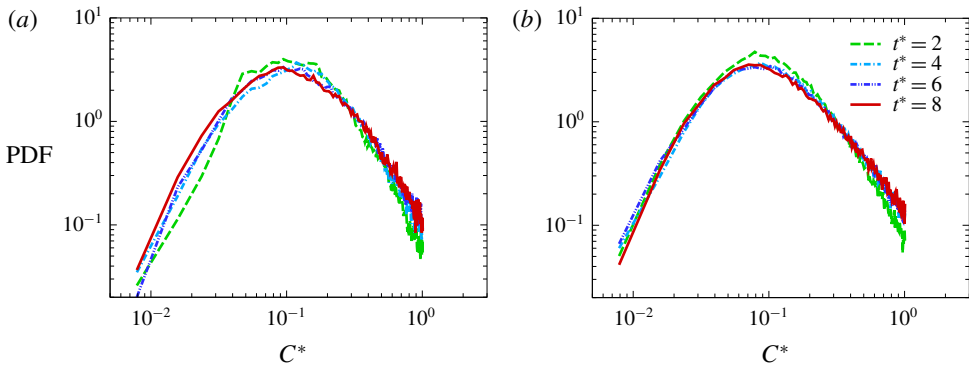


FIGURE 12. The temporal evolution of PDFs of the normalized characteristic curvature of propagating surfaces in non-reacting DNS: (a) case B and (b) case D.

3.4. Modelling of the truncation time

The determination of the truncation time scale T_s^* in (3.11) is crucial for the modelling of A_T/A_0 using Lagrangian statistics of propagating surfaces, which is similar to the critical role of characteristic time scales in statistical turbulence models (see He, Jin & Yang 2017). Based on discussions in § 3.3, T_s^* is determined when averaged geometric quantities of propagating surfaces reach the statistically stationary state. This state is an analogy to the statistically stationary A_T/A_0 of turbulent premixed flames in combustion DNS.

We observe that T_s^* varies with u'/S_L from the temporal evolution of $\langle C^* \rangle$ in figure 11, so we assume

$$T_s^* = F\left(\frac{1}{S_L^*}\right) = F\left(Re^{-1/4} \frac{u'}{S_L}\right). \tag{3.15}$$

Next, it is essential to determine the form of function F . Inspired by the modelling approach for the width of a thermal wake in turbulent dispersion (Taylor 1921) and the pressure–rate-of-strain tensor in Reynolds stress models (Launder, Reece & Rodi 1975; Pope 2000), we first determine F at some limiting values of u'/S_L at finite Re .

As $u'/S_L \rightarrow \infty$, propagating surfaces can be considered as material surfaces. According to the discussion in §3.3, there exists a universal truncation time T_∞^* (3.13) when $\langle C^* \rangle$ reaches the statistically stationary state. If F is a smooth function, (3.13) implies that

$$\lim_{u'/S_L \rightarrow \infty} \frac{dT_s^*}{d(1/S_L^*)} = 0. \quad (3.16)$$

As $u'/S_L \rightarrow 0$, we consider a laminar premixed flame with $u' = 0$ and finite S_L . Since the initial planar propagating surface cannot deform, the truncation time is

$$\lim_{u'/S_L \rightarrow 0} T_s^* = 0. \quad (3.17)$$

In weak turbulence with very small u'/S_L , the dependence of S_T on u' can be described by a general power law (e.g. Peters 1999; Creta & Matalon 2011; Lipatnikov 2012)

$$\frac{S_T}{S_L} = 1 + C \left(\frac{u'}{S_L} \right)^\zeta, \quad (3.18)$$

where C is independent of u' but may depend on the unburnt mixture composition (Lipatnikov & Chomiak 2002), and ζ is an empirical constant.

The first-order Taylor expansion of the modelled area ratio (3.11) with (3.2) for very small T_s^* and u'/S_L is

$$\frac{S_T}{S_L} = 1 + \xi T_s^*. \quad (3.19)$$

This should be consistent with (3.18) at a laminar state with $Re = 1$, so we have

$$\lim_{u'/S_L \rightarrow 0} \frac{d^n T_s^*}{d(1/S_L^*)^n} = \frac{C}{\xi} \prod_{m=0}^{n-1} (\zeta - m) \left(\frac{u'}{S_L} \right)^{\zeta-n} \quad (3.20)$$

with an integer $1 \leq n \leq \zeta$. Here, we specify $\zeta = 1$ as the simplest linear model

$$S_T = S_L + C u' \quad (3.21)$$

in weak turbulence, which is generally applicable to various fuels. Then (3.20) is simplified as

$$\lim_{u'/S_L \rightarrow 0} \frac{dT_s^*}{d(1/S_L^*)} = \frac{C}{\xi}. \quad (3.22)$$

In order to determine C , we only need a very few sample data points

$$G = \{(x_i, y_i) = (u'/S_L, S_T/S_L) \mid i \in \{0, 1, \dots, N_G\}\} \quad (3.23)$$

from existing DNS or experimental measurement of propagating flames in weak turbulence with $u'/S_L < \epsilon_c$, where the small threshold value is set to $\epsilon_c = 2$ and the data point of $(x_0, y_0) = (0, 1)$ at laminar conditions is specified. Then, a least-squared fit is utilized to estimate C from G as

$$C = \frac{\sum x_i y_i - \sum x_i \sum y_i / N_G}{\sum x_i^2 - (\sum x_i)^2 / N_G}. \quad (3.24)$$

This simple linear fit appears to be more robust than the high-order fit with $\zeta > 1$ in (3.18) from very sparse sample data points with finite uncertainties.

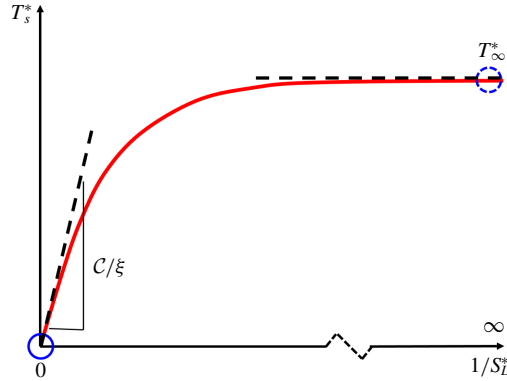


FIGURE 13. A schematic diagram for the functional form of F for T_s^* . Circles: values of F at limiting conditions (3.13) and (3.17); dashed lines: slopes of F at asymptotic conditions (3.16) and (3.22).

Considering the function F at all the limiting values above (also sketched in figure 13), we propose a model for the truncation time as

$$T_s^* = T_\infty^* \left[1 - \exp \left(-\frac{C}{\xi T_\infty^* S_L^*} \right) \right], \tag{3.25}$$

which satisfies (3.13), (3.16), (3.17) and (3.22), and is a monotonically increasing function in terms of $1/S_L^*$. It is noted that substituting the first-order Taylor expansion of (3.25) in terms of very small $1/S_L^*$ into (3.19) with $Re = 1$ recovers the linear model (3.21).

3.5. Modelling of the area growth rate

In the modelling of A_T/A_0 in (3.11), the constant ξ needs to be determined by a function of given turbulence or flame parameters. Although ξ_A grows with time in figure 10, we approximate ξ_A as a constant effective growth rate

$$\xi = \xi_A(t^* = T_\infty^*) \tag{3.26}$$

at the universal truncation time T_∞^* .

Since the growth of $A(t^*)/A_0$ is independent of Re , as demonstrated in figure 9(b), ξ at large Re should be the same for a given mixture composition. For example, we estimate $\xi = 0.35$ by (3.26) from case E of the DNS of propagating surfaces. In figure 9(b), the comparison of $A(t^*)/A_0$ from DNS and the model (3.8) with $\xi = 0.35$ indicates that (3.8) with (3.26) can provide a good approximation for the growth of $A(t^*)/A_0$.

Furthermore, ξ may vary with S_L^* for the same Re , so it is necessary to model this possible dependence of ξ on different mixture compositions or fuels. By comparing (3.11) and (3.6), we obtain

$$\xi T_s^* = \int_0^{T_s^*} \langle K_t^* \rangle_A + 2S_L^* \langle \kappa^* \rangle_A ds. \tag{3.27}$$

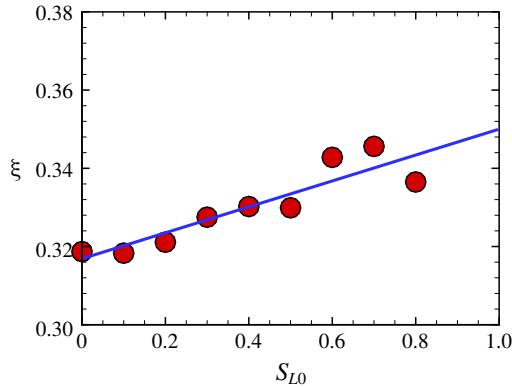


FIGURE 14. Modelled area growth rates of propagating surfaces with $S_L = 0 \sim 0.8 \text{ m s}^{-1}$ in non-reacting HIT. Circles: results obtained by (3.26) from the tracking of propagating surfaces in case E; solid line: the linear fit (3.29) with $\mathcal{A} = 0.317$ and $\mathcal{B} = 0.033$.

Applying the mean value theorem for integrals to (3.27) yields

$$\xi = \frac{1}{2} \langle K_t^*(t') \rangle_A + S_L^* \langle \kappa^*(t') \rangle_A, \quad t' \in (0, T_s^*), \quad (3.28)$$

which indicates an explicit dependence of ξ on the laminar flame speed.

Considering the independence of ξ for large Re , we use DNS case E of propagating surfaces with varying S_L to fit (3.28). We find that $\xi = 0.33 \pm 0.02$ has a weak dependence on S_L for a range of moderate S_L in figure 14, where the selection of $S_L = 0 \sim 0.8 \text{ m s}^{-1}$ covers all the S_L in the combustion DNS series discussed in § 4.1. Since the dependence appears to be linear, we propose an empirical model

$$\xi = \mathcal{A} + \mathcal{B}S_{L0}. \quad (3.29)$$

Here, model coefficients $\mathcal{A} = 0.317$ and $\mathcal{B} = 0.033$ are determined by the least-squared fit, and they represent the tangential strain-rate and propagation-curvature effects in (3.28), respectively; $S_{L0} = S_L/S_{L,ref}$ is a dimensionless laminar flame speed and is normalized by a reference value $S_{L,ref} = 1 \text{ m s}^{-1}$.

We remark that the model (3.29) can be valid for various fuels with moderate S_L , but it may break down for very large S_L . In principle, ξ of initial planar propagating surfaces is vanishing as $S_L/u' \rightarrow \infty$, so we speculate that ξ may decrease at very large S_L .

3.6. Predictive model of the turbulent burning velocity

Substituting models (3.25) for T_s^* and (3.29) for ξ into (3.11) and using (3.2), we obtain

$$\frac{S_T}{S_L} = \exp \left\{ T_\infty^* (\mathcal{A} + \mathcal{B}S_{L0}) \left[1 - \exp \left(-\frac{CRe^{-1/4}}{(\mathcal{A} + \mathcal{B}S_{L0}) T_\infty^* S_L} u' \right) \right] \right\}. \quad (3.30)$$

The physical meaning and determination method of the model parameters in (3.30) are summarized in table 3. They are either given turbulence/flame parameters or universal constants pre-determined by Lagrangian statistics of propagating surfaces, except for

Parameter	Physical meaning	Determination method
Re	Reynolds number of turbulence	Given parameter
S_{L0}	Dimensionless laminar flame speed	Given parameter
T_∞^*	Time for the stationary state of m.s.	Constant calculated from DNS of m.s.
\mathcal{A}	Tangential strain-rate effect of p.s.	Constant fitted from DNS of p.s.
\mathcal{B}	Propagation-curvature effect of p.s.	Constant fitted from DNS of p.s.
\mathcal{C}	Combustion chemistry of fuel	Fit from S_T in weak turbulence

TABLE 3. Summary of the model parameters in the proposed model (3.30), where m.s. and p.s. denote material and propagating surfaces in non-reacting HIT, respectively.

\mathcal{C} determined by (3.24) from one or a few available data points of S_T of premixed flames in weak turbulence.

The model (3.30) can predict most of the basic trends of S_T summarized in Lipatnikov & Chomiak (2002). As $u'/S_L \rightarrow 0$ with $Re = 1$, (3.30) is reduced to the linear model (3.21), so the modelled S_T increases with u' and \mathcal{C} for small u'/S_L . The form of (3.30) implies the ‘bending’ of S_T/S_L at moderate u'/S_L . As $u'/S_L \rightarrow \infty$ with finite Re , this model converges to a finite value

$$\frac{S_T}{S_L} = \exp [T_\infty^* (\mathcal{A} + \mathcal{B}S_{L0})]. \quad (3.31)$$

This implies that the modelled S_T depends weakly on u' and increases with the laminar flame speed at large u'/S_L , but it cannot predict the global quenching of flames characterized by a sharp drop of S_T/S_L at very large u'/S_L (e.g. Karpov & Severin 1978, 1980; Driscoll 2008; Lipatnikov 2012). In particular, (3.31) suggests that the assumption in (3.10) with modelled T_s^* in (3.25) recovers the finite flame area in high- Re turbulence by implicitly accounting for surface annihilation of real flames.

Substituting all the model constants $\mathcal{A} = 0.317$, $\mathcal{B} = 0.033$ and $T_\infty^* = 5.5$ calculated from Lagrangian statistics of propagating or material surfaces in non-reacting HIT, we finally obtain a predictive model for the turbulent burning velocity in terms of u'/S_L as

$$\frac{S_T}{S_L} = \exp \left\{ (1.742 + 0.182S_{L0}) \left[1 - \exp \left(-\frac{CRe^{-1/4} u'}{1.742 + 0.182S_{L0} S_L} \right) \right] \right\}. \quad (3.32)$$

This model is validated in § 4.1 by three DNS data sets of various fuels.

Compared with existing models of S_T , the features of the present one are summarized as follows. (i) The Lagrangian history of flame wrinkling is represented by the Lagrangian statistics of propagating surfaces in non-reacting HIT, and is utilized to construct the model. In other words, the model (3.30) not only depends on local values of u' , flow integral property Re and flame properties S_L and \mathcal{C} , but also on the Lagrangian-based parameters T_∞^* , \mathcal{A} and \mathcal{B} . (ii) The Re -independent profile of $A(t^*)$ in terms of the quantities normalized by Kolmogorov scales is used in the modelling procedure, which introduces the universal statistics of propagating surfaces in small-scale turbulence and naturally involves the effect of Re on S_T in terms of integral scales. (iii) All the model parameters are derived via scale analysis and asymptotic analysis, and their values are determined by DNS of propagating surfaces in non-reacting HIT and existing data of S_T in weak turbulence.

DNS series	Present DNS	Nivarti & Cant (2017)	Lee & Huh (2010)
Unburnt mixture	H ₂ /air	CH ₄ /air	Progress variable
Chemistry	Detailed	One step	One step
S_{L0}	0.727	0.39	0.0016
\mathcal{C}	2.43	0.55	1.0

TABLE 4. Summary of the model parameters in three DNS series with various fuels.

4. Model assessment

4.1. *A posteriori* test

We assess the model (3.32) of S_T by comparing the model prediction and the results from the present combustion DNS and another two DNS series in the literature (see Lee & Huh 2012; Nivarti & Cant 2017) with the same flame configuration in figure 1 but with different fuels and S_L .

The three DNS series of turbulent premixed flames are briefly reviewed below. (i) The present DNS: H₂/air flame with detailed chemistry. (ii) DNS of Nivarti & Cant (2017): CH₄/air flame with the chemistry described using a single-step Arrhenius expression. (iii) DNS (Group T) of Lee & Huh (2010): the premixed mixture is modelled by a reaction progress variable, and the chemistry is computed by the single-step Arrhenius expression. As shown in figure 2, these three DNS series cover a range of Re , Ka and premixed combustion regimes. All the model parameters in (3.32) are summarized in table 4, where \mathcal{C} for each case is calculated from one or two corresponding DNS data points of S_T at $u'/S_L < 2$ by (3.24).

The model (3.32) is validated by combustion DNS of various fuels in figure 15. In general, the model predictions (solid lines) from (3.32) agree well with the DNS results (symbols) and capture the bending of the profile of S_T/S_L in terms of u'/S_L . The overall good agreement ranges over $0 < u'/S_L \leq 20$ and various fuels, indicating the generality of our proposed model. In appendix D, the present model is also compared with other models of S_T in the three DNS series, and the present one gives the overall best performance. The discrepancies at very large u'/S_L for DNS series of Nivarti & Cant (2017) and Lee & Huh (2010) are perhaps due to the breakdown of flame fronts close to the broken reaction zone. Moreover, uncertainties of the model constants in (3.30) can result in the discrepancies, which are elaborated below.

First, the value of \mathcal{C} is fuel dependent and relies on available data points of S_T under weak turbulence. In principle, the linear scaling (3.21) is recovered at $u'/S_L = 0$ with $Re \sim O(1)$. On the other hand, if only the data points of S_T/S_L with finite u'/S_L and $Re > O(1)$ are available, \mathcal{C} fitted from (3.24) can cause the discrepancy from (3.21) near $u'/S_L = 0$ in figure 15.

Furthermore, if there are no available data of S_T/S_L for fitting \mathcal{C} , we suggest that the value of \mathcal{C} can be simply set to $\mathcal{C}_0 = 2.0$ for hydrogen fuels and $\mathcal{C}_0 = 1.0$ for other fuels based on the chemical activity of the fuels. We observe the good agreement between the DNS result and the model prediction of (3.32) with the empirical constant $\mathcal{C} = \mathcal{C}_0$ instead of fitting \mathcal{C} from data, and illustrate the sensitivity of the model prediction to \mathcal{C} by varying $\mathcal{C} = \mathcal{C}_0 \pm 0.5$ in figure 16. In general, S_T/S_L predicted from (3.32) increases with \mathcal{C} .

Second, the model constants \mathcal{A} , \mathcal{B} and T_∞^* appear to be universal, but the determination of their values may involve some uncertainties owing to numerical schemes, forcing methods and finite- Re effects in the DNS of non-reacting HIT

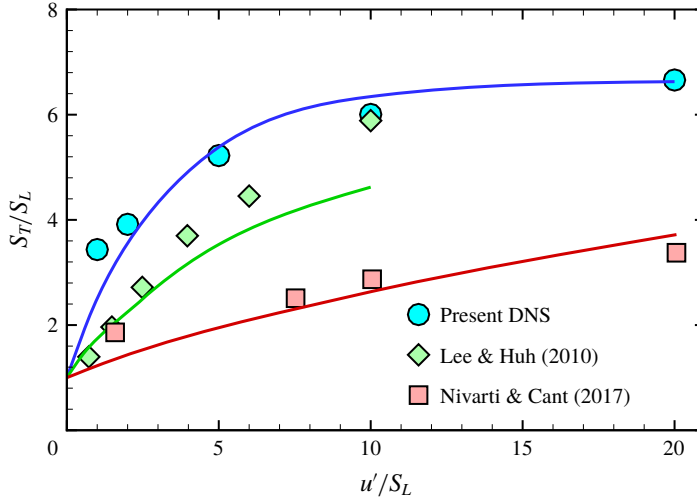


FIGURE 15. Comparison of S_T calculated from the combustion DNS (symbols) and the proposed model (3.32) (solid lines).

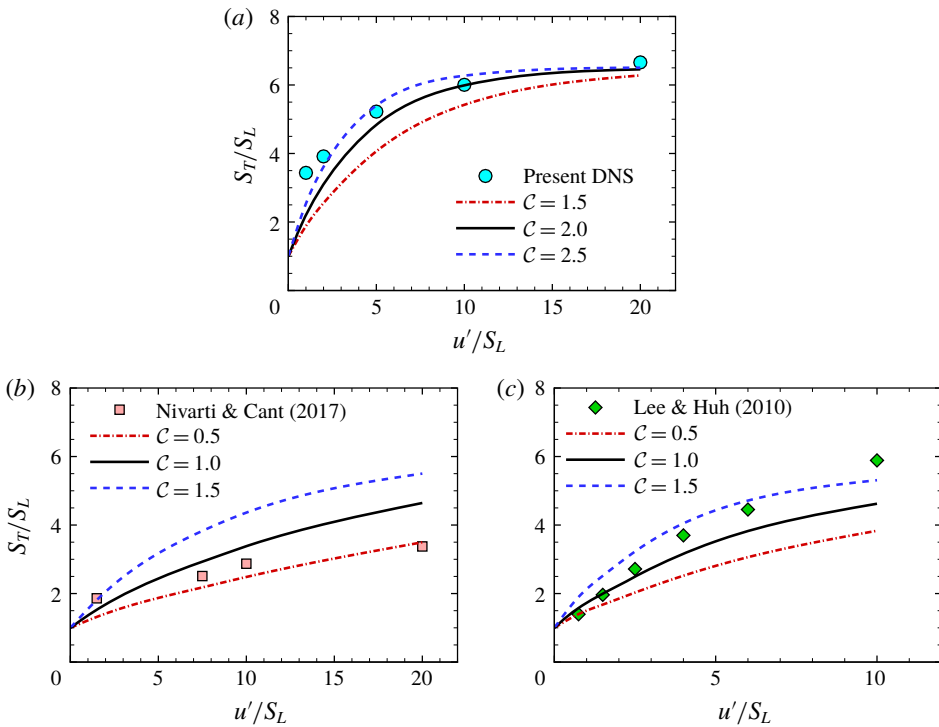


FIGURE 16. Model predictions of S_T with the model constant $C = C_0$ or $C = C_0 \pm 0.5$.

and fitting methods to determine the constants, which can slightly affect the model prediction of S_T .

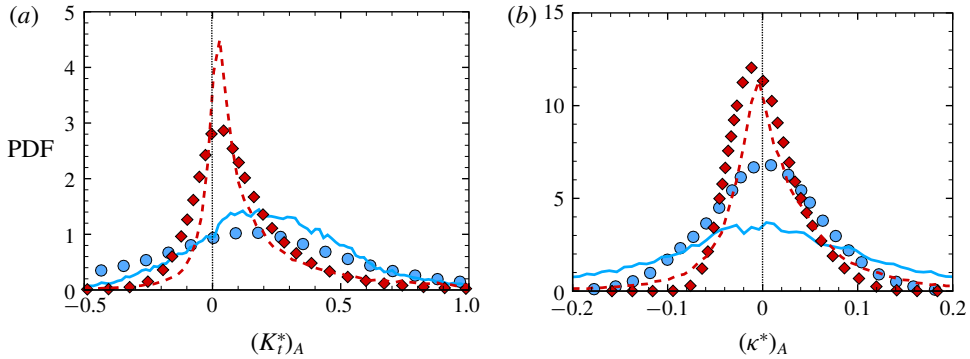


FIGURE 17. PDFs of (a) the normalized area-weighted tangential strain rate and (b) the mean curvature from flames and propagating surfaces in DNS cases B and D. Circles: flame in case B; diamonds: flame in case D; solid lines: propagating surface in case B; dashed lines: propagating surface in case D.

Although the present S_T model still has some uncertainties and discrepancies owing to the physical assumptions in model development and the lack of rigorous methods for determining \mathcal{C} , generally controlled by combustion chemistry, it is able to predict the relatively accurate bending effect for flames in HIT at large u'/S_L in figures 15 and 16, which is superior to existing S_T models (see detailed comparisons in appendix D). In particular, the propagating surface used in the model was introduced only for the flamelet regime (see Girimaji & Pope 1992), but the present modelling approach appears to extend the concept of propagating surfaces to the thin-reaction-zone regime. The truncation of the area growth by T_s^* and the cusp removal of propagating surfaces result in a finite $A(T_s^*)$, which can model the statistically stationary A_T under competing mechanisms between the flame area growth and consumption.

4.2. *A priori* test

In order to further validate the key modelling assumption in (3.10), we assess the contributions to the growth of A_T on the right-hand side of (3.6) by comparing $\langle K_t^*(T_s^*) \rangle_A$ and $\langle \kappa^*(T_s^*) \rangle_A$ of propagating surfaces at the modelled truncation time (3.25) in non-reacting HIT with $\langle K_t^* \rangle_A$ and $\langle \kappa^* \rangle_A$ of the isosurface $c = \hat{c}$ at the statistically stationary state in the present combustion DNS. The PDFs of $(K_t^*)_A$ and $(\kappa^*)_A$ from propagating surfaces and flames in two typical cases B and D are plotted in figure 17. Here, based on (3.5) and the FSD described in appendix A, $(f)_A = f\delta A/(A/N_s)$ and $(f)_A = f\Sigma'/\Sigma$ denote area-weighted quantities for propagating surfaces and flames, respectively, and $\langle f \rangle_A$ is equal to the integration of the product of $(f)_A$ and its PDF in the sample space. Moreover, K_t and κ in combustion DNS are calculated by (A 2) and (A 3).

Figure 17(a) indicates that all the cases exhibit positive $\langle K_t^* \rangle_A$, which is consistent with the positive contribution of turbulent straining to the area growth of material surfaces (Girimaji & Pope 1990). Similar PDFs of $(K_t^*)_A$ in propagating surfaces and flames imply that the straining process experienced by propagating surfaces in non-reacting HIT resembles that of flames in turbulent combustion.

Figure 17(b) shows that the PDF of $(\kappa^*)_A$ of the propagating surfaces is qualitatively similar to that of flames, but the former distribution is generally broader than the latter

one. This observation implies that nearly singular propagating surfaces with very large curvatures can be smoothed in real flames owing to diffusion and curvature effects. Furthermore, $\langle \kappa^* \rangle_A$ of flames is close to zero, which agrees with the former finding (e.g. Trouvé & Poinso 1994; Chakraborty & Cant 2005; Nivarti & Cant 2017) that the curvature effect can consume the flame area. On the other hand, $\langle \kappa^* \rangle_A$ of the propagating surfaces is slightly positive and of the order of $O(0.01)$. The cellular structures of propagating surfaces in figure 6 with positive $\langle \kappa^* \rangle_A$ (Zheng *et al.* 2017) are only observed in turbulent premixed flames at low Ka in figure 3 (see Matalon 2009), whereas they break down at high Ka . This structural difference causes the discrepancy between PDFs of $(\kappa^*)_A$ for propagating surfaces and flames in case D.

5. Conclusions

We propose a predictive model of S_T in premixed combustion in HIT based on the Lagrangian statistics of propagating surface elements in non-reacting stationary HIT. An ensemble of propagating surface elements initially constitute a plane in the non-reacting HIT to mimic the propagation of a planar premixed flame front. The effects of molecular transport and reaction on each surface element is modelled via a constant displacement speed $S_d = S_L$.

The model development involves several assumptions and modelling steps. First, S_T/S_L is approximated by the ratio A_T/A_0 of flame surface areas from Damköhler's assumption (3.2). Then, A_T/A_0 is approximated by the area ratio $A(t^*)/A_0$ of global propagating surfaces at the truncation time $t^* = T_s^*$, which signals that the characteristic curvature of initially planar propagating surfaces has reached the statistically stationary state in non-reacting HIT. This state resembles the statistical equilibrium state in combustion between the flame area growth due to turbulent straining and the area consumption due to flame self-propagation. In addition, we demonstrate that the temporal growth of $A(t^*)/A_0$ can be approximated by an exponential function (3.11) with a constant growth rate which is modelled by a linear function (3.29) of the dimensionless S_L . Accounting for T_s^* at limiting conditions of very weak and strong turbulence, we propose the model (3.25) of T_s^* by theoretical analysis and tracking of propagating surfaces. Finally, we obtain the predictive model (3.32) of S_T , an explicit expression in terms of u'/S_L and several model parameters. The model parameters include universal constants T_∞^* , \mathcal{A} and \mathcal{B} calculated from Lagrangian statistics of propagating surfaces in non-reacting HIT, and a fuel-dependent \mathcal{C} pre-determined by (3.24) from one or a few available combustion DNS or experimental data points of S_T in weak turbulence.

Being different from other models for S_T , the present one incorporates the Lagrangian information of propagating surfaces characterizing the enhancement of the area growth of flames in turbulence and the universal statistics of propagating surfaces in small-scale turbulence involving the effect of Re . Furthermore, the effect of fuel chemistry on S_T is also considered by the model parameter \mathcal{C} .

The proposed model (3.32) is validated by an *a posteriori* test against three DNS series of turbulent premixed flames in HIT, including the present combustion DNS and two in the literature, which have the same flame configuration but different fuels and S_L . The model predictions of S_T generally agree well with DNS results under a broad range of turbulent intensities and premixed combustion regimes. The expression (3.32) of the model implies that it can capture the basic trends of S_T in terms of u' , i.e. the linear growth in weak turbulence and the bending effect in strong turbulence. Furthermore, the model validity is supported by an *a priori* test.

We calculate PDFs of tangential strain-rate and propagation-curvature terms, which are two major contributions to the surface area growth, and find that the PDFs of each term in flames and propagating surfaces qualitatively agree.

On the other hand, the assumptions in the proposed model and the uncertainties in model constants cause some limitations in the model formulation and discrepancies in the model predictions, which can be improved in future work. (i) Under very strong turbulence (e.g. Aspden *et al.* 2011; Wabel *et al.* 2017), the flame can be in the broken reaction zone in which no distinct flame surface exists, so the model assumption (3.2) may be invalid. (ii) The model is developed based on the propagation of a planar flame in HIT, so it may need to be adapted for different flame configurations or geometries (Driscoll 2008). (iii) The dependence of S_T on pressure (see Lu & Yang 2019), gas expansion and differential diffusion (see Lipatnikov 2012) is not considered in the present model.

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Declaration of interests

The authors report no conflict of interest.

Supplementary material

Supplementary material is available at <https://doi.org/10.1017/jfm.2019.1081>.

Appendix A. Modelling of the FSD

In the modelling approach of FSD, the generalized local FSD $|\nabla c|$ (Veynante & Vervisch 2002) is employed to calculate the local surface-to-volume ratio $\Sigma' \equiv |\nabla c|$. The generalized FSD $\Sigma \equiv \langle \Sigma' \rangle_{c=\hat{c}}$ denotes the surface-averaged Σ' along the isosurface of $c = \hat{c}$, i.e. the flame surface-to-volume ratio in Ω .

The evolution equation of Σ (see Pope 1988; Trouvé & Poinso 1994) is

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\langle \mathbf{u} + S_d \mathbf{n} \rangle_A \Sigma) = \langle K \rangle_A \Sigma, \quad (\text{A } 1)$$

where $\mathbf{n} = -\nabla c / |\nabla c|$ denotes the flame normal, and $\langle f \rangle_A \equiv \langle f \Sigma' \rangle / \Sigma$ denotes the area-weighted average of a function f over the isosurface of $c = \hat{c}$. On the right-hand side of (A 1), the local flame stretch rate $K = K_t + 2S_d \kappa$ involves the tangential strain-rate term

$$K_t = \nabla \mathbf{u} - \mathbf{nn} : \nabla \mathbf{u} \quad (\text{A } 2)$$

and the propagation-curvature term $2S_d \kappa$ with

$$\kappa = \frac{\nabla \cdot \mathbf{n}}{2}. \quad (\text{A } 3)$$

These expressions in Eulerian coordinates are consistent with the Lagrangian formulation in (2.6). The turbulent flame area can be obtained by integrating the local FSD as

$$A_T = \int_{\Omega} \Sigma' \delta(c - \hat{c}) dV. \quad (\text{A } 4)$$

Since the turbulent burning velocity can be modelled by (3.2) with (A 4), S_T is generally increased with u'/S_L due to the increasing integration of the FSD throughout the flame brush (Nivarti & Cant 2017), but the growth of S_T can slow down or S_T can even decrease for large u'/S_L if the clear flame front is destroyed in very strong turbulence, as shown in case E in figure 3.

Appendix B. Effects of non-constant S_d on the area growth of propagating surfaces

In the DNS of propagating surfaces in non-reacting HIT, the constant displacement speed $S_d = S_L$ can be modified by including the effects of flame stretch. From the asymptotic theory, the first-order correction term for small curvature and strain rate is added as (Peters 2000; Matalon 2009)

$$S_d = S_L - \mathcal{L}K = S_L(1 - MaKaK^*), \quad (\text{B } 1)$$

where the Markstein number $Ma = \mathcal{L}/\delta_L$ denotes the ratio of the Markstein length \mathcal{L} to the laminar flame thickness δ_L and measures the sensitivity of the flame speed to the local flame stretch. For the H_2/air mixture with the equivalence ratio $\phi = 0.6$ in the present combustion DNS, we obtain $Ma = -0.18$ (see Davis & Searby 2002).

To investigate the effects of non-constant S_d , (B 1) is applied to (2.2) in the tracking of propagating surfaces in non-reacting HIT. The PDFs of S_d of propagating surfaces are evaluated at the truncation time and are compared with the combustion DNS data. Here, the displacement speed of the flame front, i.e. the isosurface of $c = \hat{c}$, is calculated by (Pope 1988)

$$S_d = \frac{\dot{\omega}_c + \nabla \cdot (\rho D_c \nabla c)}{\rho |\nabla c|}, \quad (\text{B } 2)$$

where $\dot{\omega}_c$ and D_c denote the reaction rate and the diffusivity of the progress variable in combustion DNS, respectively.

In case B with small u' , we observe that S_d is always positive from both combustion DNS and propagating surfaces. In cases D and E with larger u' , the variance of S_d increases due to the increased turbulent fluctuations experienced by the reaction layer, and the probability of negative S_d becomes higher, consistent with previous DNS results (Nivarti & Cant 2017). The PDFs of S_d from combustion DNS and propagating surfaces are qualitatively similar, which partly validates the model (B 1).

The evolutions of $A(t)/A_0$ of the propagating surfaces with constant and non-constant S_d are compared in figure 19. We find that the surface area ratios are almost identical, so the effect of non-constant S_d of (B 1) on the prediction of A_T/A_0 using propagating surfaces appears to be negligible and we only use constant $S_d = S_L$ in the model development.

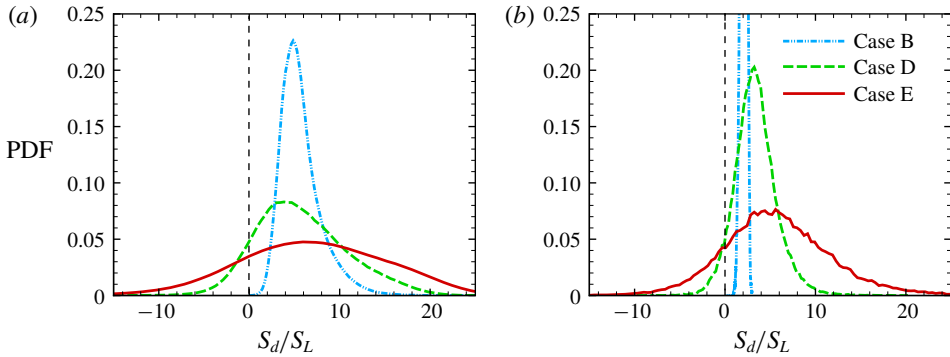


FIGURE 18. PDFs of the displacement speed for (a) flames in combustion DNS and (b) propagating surfaces in non-reacting DNS in cases B, D and E.

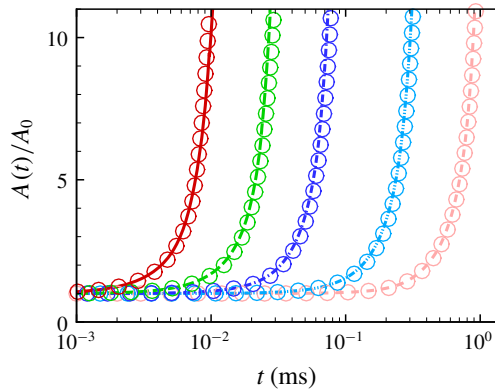


FIGURE 19. The comparison of surface area ratios of propagating surfaces with constant S_d (symbols) and non-constant S_d (lines) in cases A–E (from right to left).

Appendix C. Characteristic curvature of propagating surfaces

The governing equation of C^* can be derived from (2.4) as (see Girimaji & Pope 1992)

$$\frac{dC^*}{dt^*} = u_{3,\alpha\beta}^* g_{\alpha\beta} - (K_t^* + 2s_{\alpha\beta}^* g_{\beta\gamma} g_{\gamma\alpha}) C^* + S_d^* g_{\alpha\beta} g_{\beta\gamma} g_{\gamma\alpha} C^{*2}, \quad (C1)$$

where $g_{\alpha\beta} = h_{\alpha\beta}/C^*$ is the normalized curvature tensor of unit norm. Taking the ensemble average over $N_s(t)$ surviving surface elements in (C1) yields

$$\frac{d\langle C^* \rangle}{dt^*} = b_1 + b_2 \langle C^* \rangle + b_3 \langle C^* \rangle^2, \quad (C2)$$

where b_1 , b_2 and b_3 denote the bending, straining and propagation terms, respectively. The bending term initiates curvature on an initially planar surface, then straining and propagation effects take over. The propagation term can cause a cylindrical surface with a finite initial curvature to develop a singularity. Since b_1 , b_2 and b_3 are functions of a statistically stationary Eulerian velocity \mathbf{u} and a tensor $g_{\alpha\beta}$ of unit norm, they can be expected to be stationary random variables (Girimaji & Pope 1992).

We qualitatively analyse the exact solution to (C2) by assuming that b_1, b_2 and b_3 are constants. Since in general the turbulent straining motion produces positive mean strain rate and increases the curvature of surfaces, statistically, the stretching coefficient b_2 is negative from (C1). The surface elements are initially planar, so the initial condition for (C2) is $\langle C^*(0) \rangle = 0$.

For material surface elements with $b_3 = 0$, we have

$$\langle C^*(t^*) \rangle = \frac{b_1}{b_2} (\exp(b_2 t^*) - 1), \tag{C3}$$

with $\lim_{t^* \rightarrow \infty} \langle C^*(t^*) \rangle = b_1/|b_2|$. For propagating surfaces, we discuss solutions based on the discriminant $b_2^2 - 4b_1b_3$. If $b_2^2 - 4b_1b_3 = 0$, then we have

$$\langle C^*(t^*) \rangle = \frac{b_2^2 t^*}{2b_3(2 - b_2 t^*)}, \tag{C4}$$

with $\lim_{t^* \rightarrow \infty} \langle C^*(t^*) \rangle = |b_2|/(2b_3)$; if $b_2^2 - 4b_1b_3 \equiv \Delta_I^2 > 0$, then we have

$$\langle C^*(t^*) \rangle = 2b_1 \frac{\exp(\Delta_I t^*) - 1}{b_2 + \Delta_I - (b_2 - \Delta_I) \exp(\Delta_I t^*)}, \tag{C5}$$

with $\lim_{t^* \rightarrow \infty} \langle C^*(t^*) \rangle = 2b_1/(\Delta_I - b_2)$; if $4b_1b_3 - b_2^2 \equiv \Delta_{II}^2 > 0$, then we have

$$\langle C^*(t^*) \rangle = \frac{-b_2 + \Delta_{II} \tan \left[\frac{\Delta_{II}}{2} t^* - \arctan \left(\frac{b_2}{\Delta_{II}} \right) \right]}{b_3}, \tag{C6}$$

where $\langle C^*(t^*) \rangle$ is periodic in time but always finite.

This qualitative analysis implies that the solution to (C2) is finite as $t^* \rightarrow \infty$, which supports the occurrence of the stationary state of $\langle C^* \rangle$ shown in figure 11.

Appendix D. Comparison of model predictions of S_T

We compare the model predictions of S_T among the present model and some existing models listed below.

- (i) Linear model (3.21) with \mathcal{C} listed in table 4.
- (ii) Model suggested by Klimov (1983):

$$S_T = C_K u'^{0.7} S_L^{0.3} \quad \text{with } C_K = 1. \tag{D1}$$

- (iii) Model suggested by Zimont & Mesheriakov (1988):

$$S_T = C_Z u' Da^{1/4} \quad \text{with } C_Z = 1. \tag{D2}$$

- (iv) Model suggested by Bradley (1992):

$$\frac{S_T}{S_L} = 1 + 0.95 Le^{-1} \left(\frac{u'}{S_L} \frac{l_t}{\delta_L} \right)^{1/2}, \quad \text{with } Le = 1. \tag{D3}$$

- (v) Model suggested by Kawanabe *et al.* (1998):

$$\frac{S_T}{S_L} = 1 + 1.25 \left(\frac{u'}{S_L} \right)^{0.7}. \tag{D4}$$

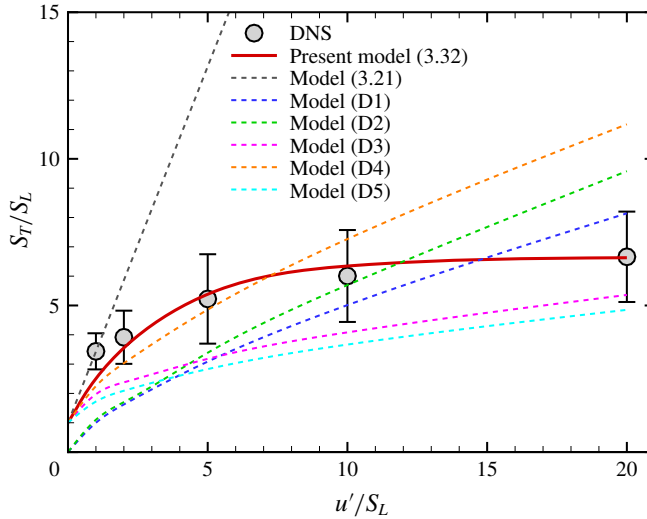


FIGURE 20. Comparison of S_T calculated from the present combustion DNS, the present model and various existing models. The error bar denotes the standard deviation of S_T/S_L in the DNS.

(vi) Model suggested by Peters (1999):

$$\frac{S_T}{S_L} = 1 + \frac{0.39}{2} \frac{l_t}{\delta_L} (\sqrt{1 + 20.5/Da} - 1). \quad (\text{D } 5)$$

Most of these models involve arbitrarily adjustable or empirical constants, and these model constants are tuned to give the best prediction of S_T for the present combustion DNS. The comparison is provided in figure 20.

We observe that the linear model is only valid for very small u' . All the other existing models can predict the trend of bending at moderate u' , but they have significant discrepancies from the DNS result, either over- or under-predictions, because these models may only be valid for certain flame/turbulence parameters and flame geometry/boundary conditions. Additionally, most of the existing models imply that $S_T/S_L \rightarrow \infty$ as $u'/S_L \rightarrow \infty$, which fails to capture the increasing bending of S_T/S_L owing to frequent local extinctions at very high Re .

We remark that the variation of instantaneous S_T is large in the present combustion DNS from the error bars in figure 20, although the mean S_T from the present DNS has been averaged over 20 large-eddy turnover times. Previous DNS studies of turbulent premixed flames (e.g. Aspden *et al.* 2011; Savard & Blanquart 2015) also observed a notable uncertainty of S_T owing to the unstable flame and the finite size of the computational domain. Thus, small discrepancies between the model prediction and DNS result should be acceptable owing to the uncertainties in the DNS result.

To further compare model performances in all the three DNS series, we define the model discrepancy as

$$\epsilon_{model} = \frac{S_T^{model} - S_T^{DNS}}{S_L}, \quad (\text{D } 6)$$

where S_T^{model} and S_T^{DNS} are obtained from models and DNS, respectively. In figure 21, the present model provides consistently good predictions for a wide range of u' and

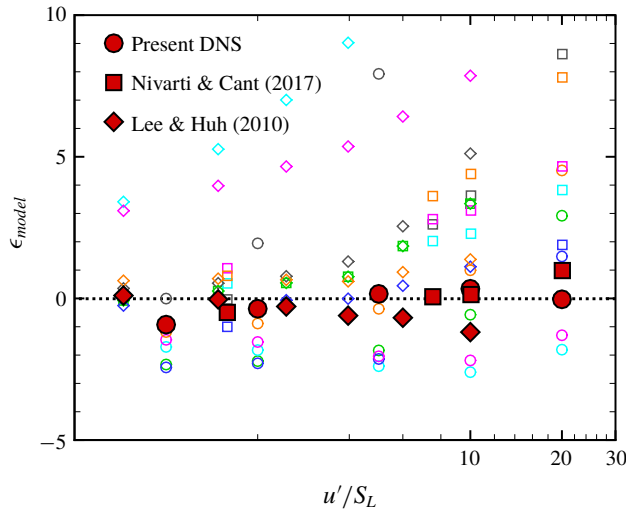


FIGURE 21. Comparison of the discrepancies from various model predictions of S_T in three DNS series. Symbols denote different DNS series. Circles: the present DNS, diamonds: Nivarti & Cant (2017), squares: Lee & Huh (2010). Colours denote different models. Red: the present model (3.32), grey: model (3.21), blue: model (D1), green: model (D2), magenta: model (D3), orange: model (D4), light blue: model (D5). The dotted line denotes $\epsilon_{model} = 0$.

various fuels, whereas other model predictions are very scattered with notable model discrepancies.

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