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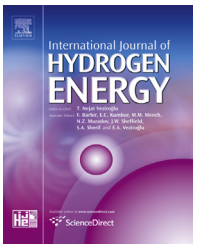

Simulation of turbulent explosion of hydrogen–air mixtures

*I. Ahmed, N. Swaminathan**

Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK

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ABSTRACT

Spherically expanding turbulent premixed hydrogen–air flames are computed using the Reynolds-Averaged Navier Stokes (RANS) approach. The mean reaction rate is modelled using unstrained and strained flamelets, and an algebraic model. Since the temperature and mass fraction evolve differently in hydrogen flames because of non-unity Lewis numbers, two reaction progress variables are used in the calculations. The computed turbulent burning velocity is compared to measured values to validate the computational models. The strained flamelets model captured the experimental variations quite well while the other two models overestimated the burning velocity of stoichiometric hydrogen–air flames. All of these models underestimated the burning velocity for a lean flame, which is thermo-diffusively unstable, indicating a need to include these instability effects in turbulent combustion modelling. A comparative analyses of stoichiometric hydrogen– and methane–air flames are also performed to understand their relative behaviour for a given turbulent combustion condition signified by u'/s_L^0 and Λ/δ. Although the gross behaviour is observed to be similar, there is a significant difference in the normalised turbulent flame speeds, s_t/s_L^0, of these flames. A detailed analysis showed that the mean reaction rate increases very sharply, at least by two orders of magnitude, near the leading edge for the hydrogen flames compared to the methane flames. Since this behaviour is controlled not only by turbulence and its interaction with flame but also by chemical kinetics, one must also consider chemical kinetics parameters such as activation temperature, in addition to u'/s_L^0 and Λ/δ to characterise s_t/s_L^0.

Introduction

The envisaged depletion of fossil fuel resources and a need to reduce pollutants emission from combustion have led to a surge in finding alternative energy sources. Hydrogen is considered as a potential future energy carrier with many benefits over the current hydrocarbon fuels [1–3]. In particular, good combustion characteristics of hydrogen make it an attractive fuel for internal combustion engines [4, 5]. Hydrogen has certain favourable combustion properties such as wide flammable range and large burning velocity, which render it as an ideal additive to improve combustion characteristics of new and bio-derived hydrocarbon fuels [6]. Also, fundamental understanding of hydrogen combustion is important from safety view points, for example generation and accumulation of hydrogen in nuclear reactors [7] and rupturing of a pressurised hydrogen storage tank can lead to explosions.

* *Corresponding author*. Tel.: +44 1223 332586.
E-mail address: ns341@cam.ac.uk (N. Swaminathan).

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Nomenclature

Roman symbols

a	flame strain rate, 1/s
c	progress variable
C_3, C_4, K_c^*	constants in the model for $\tilde{\varepsilon}_c$
C_p	mixture specific heat capacity at constant p, J/(kg K)
D	molecular diffusivity, m^2/s
Da	Damköhler number
D_t	turbulent diffusivity, m^2/s
k	turbulent kinetic energy, m^2/s^2
Ka	Karlovitz number
K	stretch factor
Le	Lewis number
M	mixture molecular weight
m_f	fuel mass, kg
N	instantaneous scalar dissipation rate, 1/s
$\boldsymbol{n}$	unit normal vector to the flame
p	pressure, Pa
Q_{LHV}	lower heating value, J/kg
Q	heat release, J
r	radial distance, m
r_f	flame radius, m
Re_t	turbulence Reynolds number
s_c	consumption speed, m/s
s_L^0	unstrained laminar flame speed, m/s
s_d	flame displacement speed, m/s
s_t	turbulent flame speed, m/s
T	temperature, K
t	time, s
t_c	chemical time, s
u_t	turbulent burning velocity, m/s

Calligraphic symbols

$\mathscr{D}$	molecular diffusivity of c, m^2/s
$\mathscr{L}$	Markstein length

Greek symbols

β'	constant in the model for $\tilde{\varepsilon}_c$
δ	chemical length scale, Zeldövich flame thickness, m
δ_L^0	laminar thermal thickness, m
δ_t	turbulent flame brush thickness, m
ε_c	scalar dissipation rate of c, 1/s
ε	dissipation rate of turbulent kinetic energy, m^2/s^3
κ	flame stretch rate, 1/s
Λ	turbulence integral length scale, m
ν	kinematic viscosity, m^2/s
ϕ	equivalence ratio
ψ	sample space variable for N
ρ	fluid density, kg/m^3
σ_c^2	variance of c
τ	heat release parameter
$\dot{\omega}_c$	mass reaction rate of c, kg/m^3 s
$\dot{\omega}_T$	combustion normalised heat release rate, kg/m^3 s
ζ	sample space variable for c

Superscripts

$''$	Favre fluctuation
$\sim$	Favre mean
$+$	normalised using planar laminar flame quantities
$'$	rms of Reynolds fluctuation

Subscripts

b	burnt mixture value
u	unburnt mixture value

A spherically expanding flame is commonly used to investigate fundamental characteristics of hydrogen–air combustion from various view points and these studies related to internal combustion engines [5] and safety aspects [8,9] have been reviewed in the past. This flame configuration has also been used to measure laminar burning velocity, s_L^0, and the influence of fluid dynamic stretch, κ, on flame propagation has been ignored in some of those earlier studies. This influence is typically given by $s_L = s_L^0 - \kappa\mathscr{L}$ for small values of κ and the Markstein length scale $\mathscr{L}$ can be positive or negative [10]. The stretch rate is defined as the rate of change of flame area per unit area, A, ie., $\kappa = (dA/dt)/A$ and it is given as $\kappa = (2/r_f)(dr_f/dt)$, for a spherically expanding flame of radius r_f [10]. Later studies [11–18] showed that the stretch effects must be included in the analysis to explain the presence of cellular instabilities observed in experiments of lean hydrogen–air spherical flames. The additional flame area resulting from this instability led to an increase in s_L implying a negative $\mathscr{L}$ for thermo-diffusively unstable lean hydrogen–air mixtures. The stoichiometric and rich mixtures showed positive $\mathscr{L}$.

Since the thermo-diffusive instabilities result from differential and/or preferential diffusion phenomena, the Lewis number, defined as the ratio of thermal to mass diffusivity of a deficient reactant in the mixture, is typically used to identify thermo-diffusively unstable mixtures. Lewis number is typically less than unity for lean hydrogen–air mixtures [10] and these flames are more susceptible to cellular instability [15,18–20]. A review of these studies on thermo-diffusive instabilities can be found in Ref. [21].

Turbulent spherical hydrogen–air flames have been investigated using fan-stirred bombs [20,22–25] and wind tunnels with grid turbulence [26,27] to address the role of turbulence since practical combustion invariably includes turbulence. These studies showed that the turbulent burning velocity is increased when the reactant mixture yields thermo-diffusively unstable flames and this effect is pronounced when the turbulence is weak. Accounting for thermo-diffusive instability effects in turbulent combustion modelling is a challenging task and is still an open question although some attempts has been made in the past to include hydrodynamic instability effects [28]. One way to account for thermo-diffusive instability effects is to use an effective Lewis number to modify the turbulent burning velocity expressions as has been done in [29] for hydrocarbon flames. An alternative approach is to include the instability effects in laminar flame speed correlations obtained using spherically expanding laminar flames and use them as input to turbulent combustion models based on turbulent burning velocity or flame

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