ParCFD2024
35^{th} International Conference on Parallel Computational Fluid Dynamics
Sep. 02-04, 2024, Bonn, Germany

DNS of a Hydrogen Flame Interacting With Homogeneous Isotropic Turbulence Maintained by a Deterministic Force

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ARTICLE INFO[†]

Keywords:
Premixed Hydrogen Flame;
Homogeneous Isotropic Turbulence;
Deterministic Force

ABSTRACT

Studying the interplay between a hydrogen flame and turbulence is crucial for the advancement of next-generation carbon-neutral combustion systems. In our present work, we conduct a series of direct numerical simulations (DNS) to investigate the dynamics of a premixed hydrogen flame interacting with the compressible homogeneous isotropic turbulence (HIT) maintained by a deterministic force under different pressure and turbulence intensity. Under this particular forcing method applied to turbulence at large scales, the relationship between the forcing intensity and the resulting fluctuating velocity aligns well with the experimental results. In our study, we compared the normalized turbulent burning velocity of hydrogen flames under different conditions, verified the common occurrence of bending effects at elevated pressures and validated existed turbulent burning velocity models. To further explore the dynamics of the HIT-flame interaction and fully leverage the advantages of high-precision direct numerical simulations, we analyzed several flame behaviors such as stretch and instability. The probability density functions (PDF) for the tangential strain rate and curvature are displayed and the results indicate a strong correlation between the flame surface structure and the turbulence generated by the large-scale forcing.

1. Introduction

Hydrogen energy has always been crucial for low-carbon combustion. To better utilize hydrogen energy, it's essential to explore the combustion mechanisms of hydrogen, especially its combustion characteristics in turbulent flow. Direct Numerical Simulation (DNS) can provide detailed insights into combustion and flow dynamics. Song et al. analyzed statistics of flame speed and diffusion effects of turbulent hydrogen flame [1, 2]. Lu and Yang carried out a series of DNS of lean H_2-air turbulent flames and proposed a turbulent burning velocity model [3, 4]. Building upon these previous works, we developed a turbulent forcing method adapted to our inhouse compressible solver. We used this method to compute turbulent premixed flames under different pressures and turbulence intensities, investigating physical phenomena and validating turbulent burning velocity models.

[†] This paper is part of the ParCFD 2024 Proceedings. A recording of the presentation is available on YouTube. The DOI of this document is 10.34734/FZJ-2025-02450 and of the Proceedings 10.34734/FZJ-2025-02175.

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2. Numerical methods

Our simulations are conducted using an in-house finite-difference code, Advanced flow Simulator for Turbulence Research (ASTR), which has been used for several previous studies [5, 6, 7].

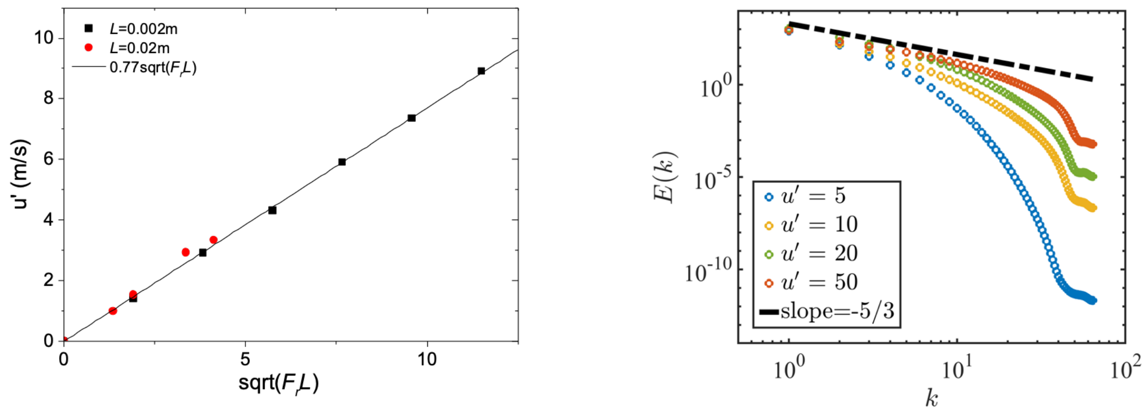
2.1. Forcing method

To maintain isotropic turbulence in our computations, we need to apply forcing to sustain turbulent fluctuations. Here, we have developed a large-scale forcing method adapted to our solver. This forcing method applies random forces to our cells in the form of sine and cosine functions within the computational domain, which is a cubic box L^3, while fixing $F_c = 0$ to ensure divergence-free conditions. The magnitude of forcing is controlled by an initially given parameter F_r for our code. The quantities ϖ_{ij} and ω_{ij} are two random variables ranging from $[-1, 1]$. The equations to solve are

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p = \mu\nabla^2\boldsymbol{u} + \frac{1}{3}\mu\nabla(\nabla\cdot\boldsymbol{u}) + \rho\boldsymbol{f}, \quad (1)$$

$$f_i = a_{ij}\sin\left(2\pi\frac{x_j}{L}\right) + b_{ij}\cos\left(2\pi\frac{x_j}{L}\right), \quad (2)$$

$$a_{ij} = \begin{cases} F_r\varpi_{ij} & i- \neq -j \\ F_c\varpi_{ij} & i = j \end{cases}, b_{ij} = \begin{cases} F_r\omega_{ij} & i- \neq -j \\ F_c\omega_{ij} & i = j \end{cases}. \quad (3)$$



(a)

(b)

Figure 1: (a) Relationship between u' and $\sqrt{F_r L}$ in different computing domain. (b) Turbulent spectra with different u'.

Figure 1a shows the linear relationship between $\sqrt{F_r L}$ and rms velocity fluctuation u' obtained with our forcing method. Figure 1b shows the turbulence spectra with different u', observing that the turbulence spectra align closely with the -5/3 power law.

2.2. Case configurations

Figure 2 presents our case setup. $L_y = L_z = 5.3\delta_L$ (flame thickness), $L_x = 8L_y$. This implies that when we choose different flame thicknesses (e.g., different pressures) for our cases, the computational domain size will change accordingly with the flame thickness variation. The domain is discretized on uniform grid points $N_x \times N_y \times N_z = 12N \times N \times N$. The numerical resolution in all the cases is ensured to resolve the smallest turbulent and flame length scales by the criterion $k_{max}\eta \geq 1.5$ and a minimum of 24 grid points within a flame thickness δ_L, respectively, where $k_{max} = \pi N/L$ is the maximum wave number magnitude in DNS of HIT and η is the Kolmogorov length scale. To meet the criteria, we set $N = 128$ for all our cases. For a specific case, we first compute a laminar one-dimensional premixed flame and scale the state variables profile of the flame surface into the three-dimensional space mentioned above, positioning the flame surface near the outlet. Then, we set up eight turbulent boxes in the x direction with the desired fluctuating velocity already evolved. This initialization aims to minimize the initial time required for reaching the statistically steady state. Eight cases are conducted with $p = 2, 5$ atm and $u'/S_L = 2, 5, 10, 20$.

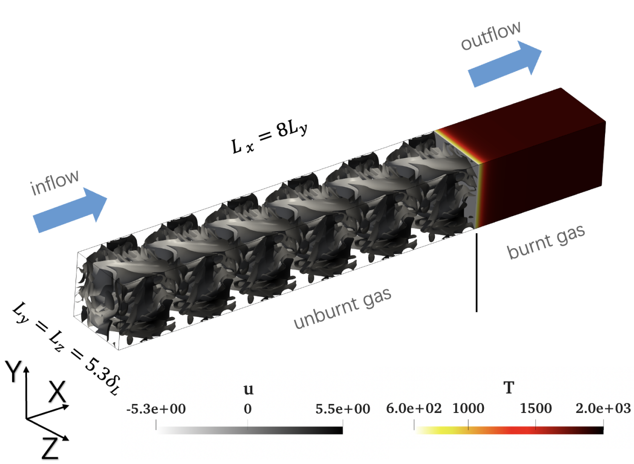


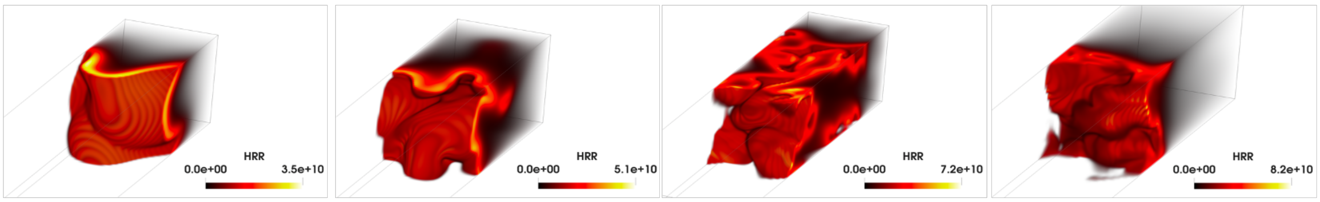
Figure 2: Initial configuration for cases. Iso-surface of vorticity is shown within the grey region and visualized by u magnitude.

3. Results and discussion

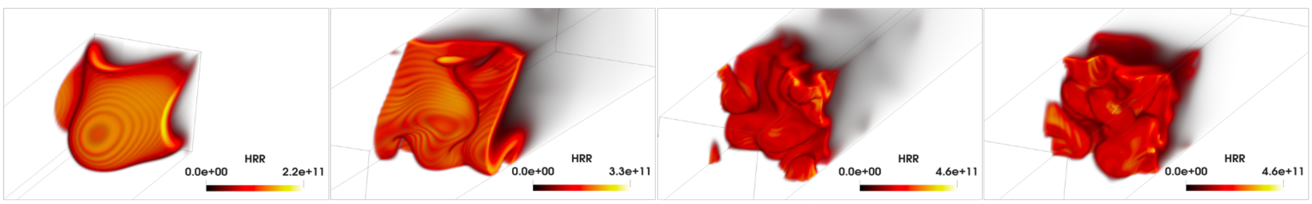
Figure 3 shows the comparison of the flame surface structures after reaching statistical steady state through displaying the isovolume of heat release rate among the cases. The upper line shows the 2 atm cases and the bottom line shows the 5 atm cases. $u'/S_L = 2, 5, 10, 20$ from left to right column. It can be observed that, in cases with the same pressure, as the turbulence intensity increases, the wrinkling of the flame surface also increases. The heat release rate in high-pressure cases is higher than that in low-pressure cases which matches our expectations.

We calculated the statistical burning velocity of our cases and compared them with the S_T model and observed the expected bending effect phenomenon as shown in Fig. 4. The turbulent burning velocity

$$s_T = \frac{1}{\rho_u Y_{\mathrm{F},u} A_L \left(t_2 - t_1\right)} \int_{t_1}^{t_2} \int_{\Omega} -\dot{\omega}_{\mathrm{F}} dV dt \qquad (4)$$

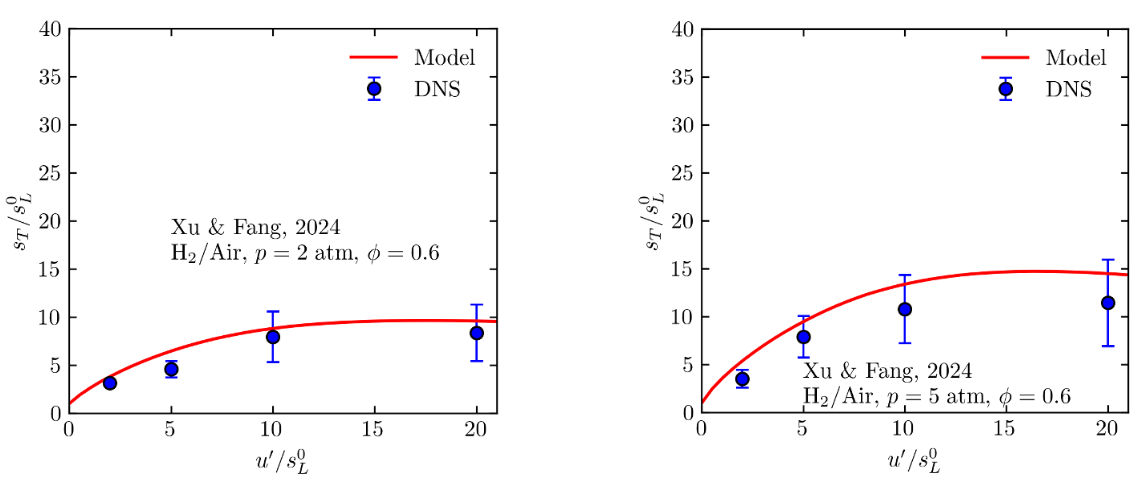


(a) $p = 2$ atm; $u'/S_L = 2, 5, 10, 20$



(b) $p = 5$ atm; $u'/S_L = 2, 5, 10, 20$

Figure 3: Flame surface structures displayed by the isovolume of heat release rate for different pressures p.



(a) (b)

Figure 4: Comparison of S_T calculated from DNS and the model.

is defined by the consumption speed. We found that our results generally align well with the Lu and Yang model [3]. This overall validation confirms the rationality of our forcing method and the accuracy of our results.

4. Conclusions

We developed a deterministic forcing method to maintain statistically stationary isotropic turbulence for studying flame/turbulence interaction. By using the deterministic forcing method and the high-order solver, we studied the hydrogen flame/turbulence interaction at different turbulence intensity and pressure. The bending curves of turbulence burning velocity are observed in our cases and the results agree well with the model proposed.

Acknowledgements

JF and XG gratefully acknowledges the support from the Computational Science Centre for Research Communities (CoSeC) and Royal Society (IEC/NSFC/223421). All the simulations were conducted on ARCHER2 and the computing time was award through the UK Turbulence Consortium (EP/R029326/1 and EP/X035484/1).

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