Flamelet-Based Modeling of Thermo-diffusively Unstable Hydrogen-Air Flames

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Abstract
Lean hydrogen-air flames morphology and propagation are highly sensitive to the onset of thermodiffusive instabilities caused by their low effective Lewis numbers. This study presents a comparative analysis of two Flamelet Generated Manifold (FGM) strategies and a data-driven modeling approach for capturing such effects and reproducing the unstable laminar flame propagation. The FGM tables differ in their choice of transported variables: one employs the mass fractions of H_2 and H_2O, while the other substitutes H_2O with the elemental hydrogen mass fraction, Z_H. Both include mixture-averaged transport and Soret diffusion. The data-driven table is derived from a reference DNS using a neural network trained to reconstruct thermochemical quantities. Model performance is assessed against DNS data, with particular focus on intrinsic instability characteristics, measured by means of the dispersion relation.

Introduction
Hydrogen-air flames pose considerable modeling challenges, particularly under lean premixed conditions. These mixtures exhibit strong susceptibility to intrinsic instabilities driven by both hydrodynamic (Darrieus–Landau) and thermodiffusive mechanisms due to their low effective Lewis numbers [1]. Capturing these instabilities accurately is essential, as they strongly influence flame propagation, structure, and overall performance in practical systems. Tabulated chemistry approaches like Flamelet Generated Manifolds (FGMs) offer a balance between computational cost and accuracy. Recent developments in data-driven modeling introduce an alternative paradigm, where high-fidelity simulations can be used for low-dimensional manifold representations capable of capturing complex flame dynamics [2].
In this context, the present study provides a comparative evaluation of two FGM strategies, differentiated by their choice of progress variables, and a data-driven approach based on a neural network trained on direct numerical simulation (DNS) data. Special attention is given to the role of preferential diffusion and the Soret effect. The objective is to assess each model's ability to reproduce the characteristic features of thermodiffusively unstable lean hydrogen-air flames.

Methodology and Results
Three distinct sets of tables were developed: two utilizing FGM and one derived from a data-driven framework. A reference DNS at $\varphi = 0.475$ was used for

comparison and to generate the data-driven table. The data-driven table was constructed by training over the DNS data through the use of a Multilayer Perceptron (MLP). The MLP optimizes a Mean Squared Error loss function through the AdamW optimizer. The hyperparameters were determined through a Random Search procedure, while training epochs were determined by the Early Stopping procedure. The FGM tables were generated with Cantera using un-stretched 1D premixed flames covering equivalence ratios from φ = 0.2 to 0.695, to account for local variations due to thermodiffusive instabilities. The first class of tables employed progress variables based on H_2 and H_2O mass fractions, while the second used a progress variable based on H_2 and the elemental mass fraction of hydrogen, Z_H. For the data-driven table, only the H_2 and H_2O-based progress variables were considered.

Following the approach adopted in [3], the transport equations solved for the controlling variables read:

$$\rho\left(\frac{\partial C_n}{\partial t}+u\cdot\nabla C_n\right)=\sum_{j=1}^{N}\nabla\cdot\left[\rho\left(D_{eff,C_nC_j}-D_{C,C_nC_j}-D_{T,C_nC_j}\right)\nabla C_j\right]+\dot{\omega}_{C_n} \quad (1)$$

Where C_n represent the N progress variables, ρ the mixture density, $\dot{\omega}_{C_n}$ the progress variable source term, and the diffusion terms represent the effective diffusion effects $D_{eff,CnCj}$, the velocity correction terms $D_{C,CnCj}$, and the Soret effect $D_{T,CnCj}$. Further clarification on the notation can be found in [3]. For the two FGM cases, three sets of simulations were performed. The first included only the effective diffusion terms $D_{eff,CnCj}$; the second added the Soret diffusion contributions $D_{T,CnCj}$; and the third further incorporated the velocity correction terms $D_{C,CnCj}$. In contrast, the data-driven approach considered only the effective diffusion terms. All simulations were carried out using an in-house solver based on the OpeFOAM suite [2]. The computational grid was resolved with 20 points across the flame thickness, consistent with the reference DNS.

Figure 1 presents the dispersion relation for the various modeling approaches, compared against the reference DNS. The data-driven model, despite excluding Soret

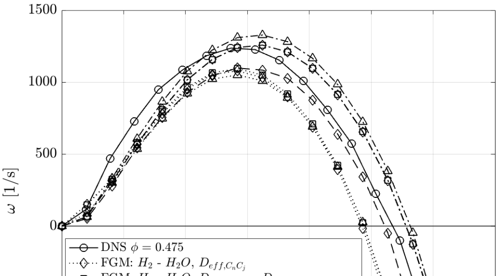

Figure 1. Dispersion relation comparison

and velocity correction terms in the transport equations, accurately captures the cutoff wavelength, but underpredicts the peak growth rate ω. The FGM model using H_2 and H_2O slightly overestimates both the cutoff and the peak, whereas the formulation with H_2 and Z_H slightly underestimates them. The impact of including Soret and velocity correction terms is more pronounced for the H_2–H_2O-based FGM approach, leading to noticeable shifts in the dispersion curve. In contrast, these effects have minimal influence when using H_2 and Z_H as progress variables, indicating lower sensitivity to detailed transport in that formulation.
Figure 2 shows the source term fields obtained using the different modeling approaches compared with the reference DNS. The figure illustrates that both methodologies successfully reproduce the key structural features characteristic of wrinkled thermo-diffusively unstable flames.

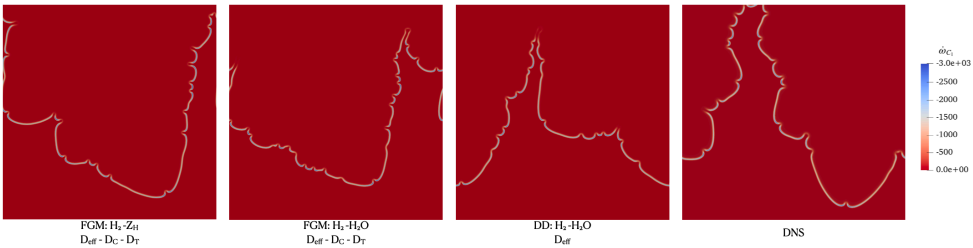

Figure 2. Source term fields comparison in the non linear regime.

Conclusion

This study compares FGM and data-driven models for thermodiffusively unstable lean H_2-air flames. The data-driven approach captures cutoff wavelengths well but underestimates peak growth rates. Among FGM strategies, using elemental hydrogen (Z_H) offers lower sensitivity to transport effects and good predictive accuracy. Including Soret and velocity corrections influences the H_2–H_2O formulation more than the Z_H-based one. All modeling approaches seem to capture correctly the behavior of thermo-diffusively unstable flames in the non-linear regime.

References

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