A DATA-DRIVEN APPROACH FOR HYDROGEN PREMIXED COMBUSTION MODELING

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Abstract

Lean premixed hydrogen flames are characterized by the high mobility of the hydrogen molecule that yields mixtures with an effective sub-unity Lewis number. This causes formation of intrinsic instabilities as a consequence of the hydrodynamic and thermo-diffusive mechanisms. The interaction of these instabilities leads to complex and non-linear corrugations of the flame front, even in laminar fla-mes, with characteristic length-scales falling under the subgrid level, requiring therefore dedicated modeling when approaching the flame to LES. In this contribution, a data-driven model for lean premixed hydrogen combustion is presented. It consists in a two-scalars manifold representation, obtained by the spatial filtering of a two-dimensional, fully resolved, unstable, self-wrinkling DNS hydrogen/air dataset. The method is validated a-priori and a-posteriori against a two-dimensional DNS.

Introduction

Hydrogen combustion is a promising alternative to fossil fuels due to its sustainability characteristics [1]. Due to the higher adiabatic flame temperatures of hydrogen, leaner mixtures are employed compared to conventional fuels. Hydrogen combustion is characterized by the high mobility of the hydrogen molecule that causes the mixture Lewis number to decrease under sub-unity values. Under such condition, particularly crucial for lean mixtures, the flame is prone to develop combustion instabilities [2] since small-scale perturbations are amplified leading to the formation on self-wrinkled unstable cellular structures [3]. These are caused by the local perturbations of the flame speed as a consequence to the local imbalance between the thermal conductivity of the mixture and the molecular diffusivity of the controlling reactant, with a mechanism known as thermo-diffusive instability [4]. In addition, these can be enhanced by the interaction with the large-scale hydrodynamic (or Darrieus-Landau) instabilities, which cause the further corrugation of the flame front as a consequence of the thermal expansion [5]. The flame propagation is significantly affected by the interaction of such instability mechanisms, resulting in the formation of non-linear multi-scale self-wrinkling structures that are largely different from the laminar one-dimensional flame structure. The smallest flame front

corrugations are of the order of the flame thickness, and require therefore dedicated modeling when resorting to the LES framework, with the twofold aim of reproducing the flame structure and accounting for the cellular wrinkling falling at the LES subgrid level even in a laminar setting [6,7]. Models for the turbulence-chemistry inter-action are usually sought, in this context, to reduce the computational cost associ-ated to the solution of the reactive chemistry. Among these, tabulated chemistry approaches are used to represent the thermo-chemical properties on lower-dimen-sional manifolds defined by a few conserved scalars, whose transport equations are solved at run time. For what concerns hydrogen premixed combustion, it has been shown that at least two scalars are needed to have a sufficiently accurate representation of the complex multi-scale, unsteady, stretched character of thermo-diffusively unstable flames, with a significant accuracy improvement with respect to the one-dimensional manifolds found in literature [7,8,9]. In the work by Lapenna et al. [7], the manifold parameterization is given as a function of the non-dimensional temperature Θ and the deficient reactant mass fraction Y_{H2}. Regele et al., instead, presented a manifold parameterized as a function of the progress variable C, based on the water mass fraction, and of the mixture fraction Z [8].

Theoretical formulation

The model presented in this work targets the modeling of unstable self-wrinkling lean hydrogen premixed flames, in a laminar setting, through a manifold representation using as defining scalars two species mass fractions, namely Y_{H2} and $Y_{H2O.}$ The model is based on the F-TACLES method, which is one of the original implementations of the tabulated approaches [10]. Both the models are based on the spatial filtering of a detailed flame solution, in order to recover all the filtered quantities as functions of the filtered progress variable, with the advantage of retaining by construction the original stretched laminar flame speed also in absence of the turbulence leading to subgrid wrinkling [10]. While the F-TACLES approach uses a 1D flame solution as source for the filtering procedure, the approach proposed in the present work employs instead a fully resolved, 2D, unstable, self-wrinkling flame [7]. Such flames are chosen since it has been demonstrated that 2D flames subject to hydrodynamic instabilities present most of the morphological features of the corresponding 3D large-scale flames [11]. The model aims in particular at using the smallest scale DNS which presents the formation of at least one of the characteristic structures of the large-scale target flame. The DNS used in this work belong to the multi-step chemistry hydrogen/air dataset by Berger et al. [4], consisting of statistically planar premixed flames, two realizations are shown in Fig. 1. In particular, a large-scale DNS with a cross-wise dimension $L_x = 800\ \ell_T$, will be considered as target flame in the following, while a small-scale flame with $L_x = 50\ell_T$, will be used as source for the filtering procedure. In both cases, the stream-wise dimension is $L_y = 200\ell_{T,}$ where $\ell_{T\ is}$ the laminar thermal flame thickness of a 1D unstretched flame. The unburned mixture features

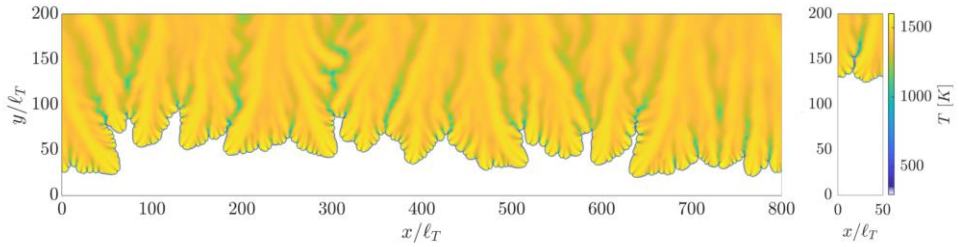

Figure 1. Temperature field in the DNS dataset [4].

an equivalence ratio of φ = 0.4, an unburned temperature of T_u = 298 K and a pressure of p = 1 bar.
The chosen scalars are normalized in order to retrieve two progress variables as shown in Eq. (1), where the subscripts *min* and *max* refer respectively to the minimum and maximum values of the corresponding mass fraction found in the employed dataset.

$$C_1 = 1 - \frac{Y_{H2} - Y_{H2,min}}{Y_{H2,max} - Y_{H2,min}} \quad C_2 = \frac{Y_{H2O} - Y_{H2O,min}}{Y_{H2O,max} - Y_{H2O,min}} \tag{1}$$

The transport equations for the two chosen manifold parameters read:

$$\frac{\partial}{\partial t}\left(\rho C_{1,2}\right) + \nabla \cdot \left(\rho u C_{1,2}\right) = \nabla \cdot \left(\rho D_{1,2} \nabla C_{1,2}\right) + \dot{\omega}_{C_{1,2}} \tag{2}$$

Where ρ is the density, D the diffusivity and $\dot{\omega}$ the scalar source term. The LES equations are obtained from Eq. (2) by means of filtering:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{C}_{1,2}\right) + \nabla \cdot \left(\bar{\rho}\tilde{u}\tilde{C}_{1,2}\right) = \nabla \cdot \left(\overline{\rho D_{1,2} \nabla C_{1,2}}\right) - \nabla \cdot \left(\bar{\rho} u \tilde{C}_{1,2} - \bar{\rho}\tilde{u}\tilde{C}_{1,2}\right) + \overline{\dot{\omega}}_{C_{1,2}} \tag{3}$$

where – operator and ~ operator respectively represent the spatial filtering and the density-weighted filtering operation. The *unfiltered* tabulated manifold is obtained by calculating for each thermochemical quantity in Eq. (2) the conditional average with respect to the two unfiltered parameters from the small-scale DNS shown in Fig. 1, which, for a generic quantity ψ is $\psi = \langle \psi | C_1, C_2 \rangle$. In order to obtain the *filtered* tabulated manifold, the source DNS must be filtered with a Gaussian filter whose size is representative of a LES grid size, as shown in Fig. 2. The thermochemical properties and unclosed terms of Eq. (3) will be therefore calculated as $\tilde{\psi} = \langle \psi | \tilde{C}_1, \tilde{C}_2 \rangle$. Figure 3 reports two examples of the obtained tables.

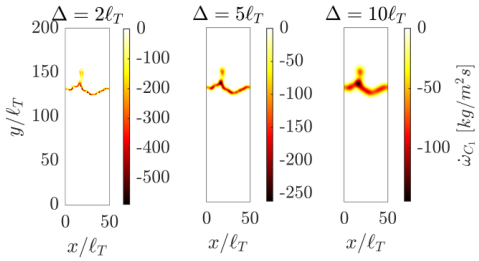

Figure 2. C_1 source term in the filtered small-scale DNS at several filter sizes.

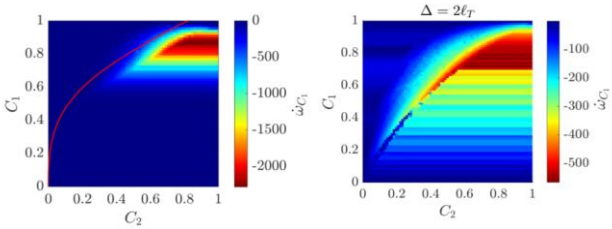

Figure 3. Unfiltered (left) and filtered (right) tables for the C_1 source term.

Results

The model is first validated *a-priori* comparing the unfiltered/filtered target DNS field with the field built accessing the unfiltered/filtered manifold with the state of the target flame. The analysis has been conducted for both the unfiltered and filtered manifolds, Fig. 4 shows a qualitative comparison performed on the first scalar source term $\dot{\omega}_{C_1}$ for the filtered case employing several filter sizes shown before. For the sake of conciseness only portions of the large-scale filtered fields have been reported. It is found that the model reproduces satisfactorily the filtered large-scale DNS for all the filter sizes, with some minor differences in the peak values reconstruction for the largest filter size. Figure 5 reports a quantitative comparison in terms of normalized consumption speed $S_C = \frac{-1}{L_y \rho_u} \int \dot{\omega_{C_1}} dxdy$ between the filtered large-scale target DNS and the fields obtained from the manifolds. It is observed that the error on the prediction increases with the filter size, with a maximum error lower than ~13%.

The unfiltered manifold is then tested *a-posteriori* performing the numerical simulation of the small-scale DNS retrieving all the thermochemical quantities needed in Eq. (2) from the unfiltered manifold. The numerical domain employed is equivalent to the DNS one. The simulation is started with a uniform unstretched solution, to which is added an initial sinusoidal disturbance in order to trigger instability formation. The flame propagation responds to the initial perturbation with a corrugation of the flame front characterized by a wavelength of ~6 ℓ_T in agreement with the linear stability analysis performed in [4]. The initial corrugation is then enhanced up to the formation of the large-scale unstable structure reported

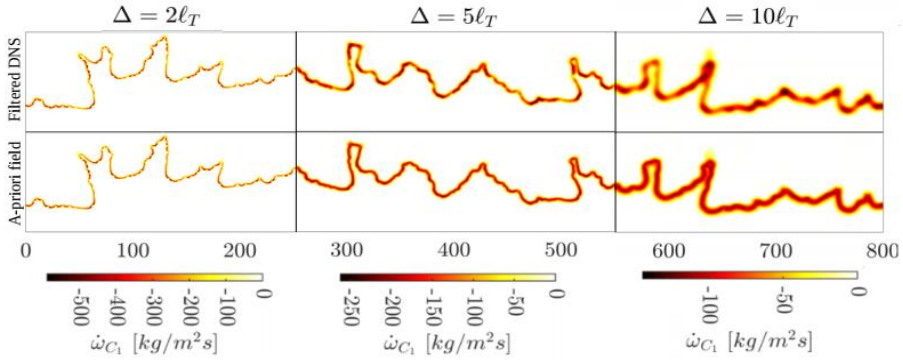

Figure 4. Comparison between the filtered DNS (top) and the a-priori field built from the filtered manifolds (bottom) for different filter sizes.

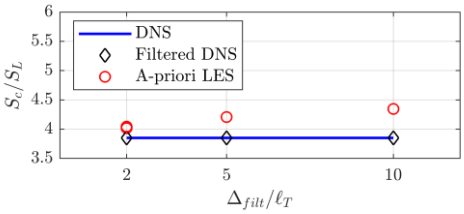

Figure 5. Consumption speeds from the a-priori analysis of the filtered manifold.

in Fig. 6, showing that the model is capable of qualitatively predicting the self-wrinkling of a thermo-diffusively unstable flame. The quantitative comparison in terms of consumption speeds results for the unfiltered setting in an error of ~2.4%.

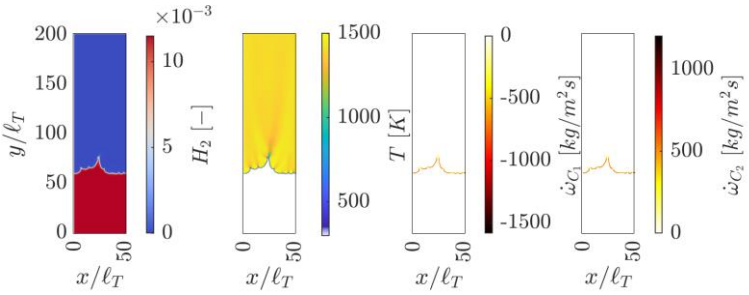

Figure 6. *A-posteriori* unfiltered simulation.

Conclusions

This work proposes a data-driven approach for lean premixed hydrogen combustion. The model is based on a two-scalars manifold representation obtained through the spatial filtering of a fully-resolved, two-dimensional, thermo-diffusively unsta-

ble flame. A set of two-dimensional tables has been developed both in an unfilte-red and filtered setting, using for the latter three different filter sizes representative of as many LES grid sizes. The *a-priori* validation of the model has shown that it correctly reproduces the morphological features of the large-scale target field and satisfactorily retains the consumption speed value with a small error for the largest filter size. The *a-posteriori* validation of the unfiltered tabulation has shown promising results in terms of prediction of the self-wrinkling nature of the thermo-diffusive flames and the formation of its characteristic instabilities.

Acknowledgments

This work is partially supported by the Italian Ministry of University and Research (MUR) and by Lazio-Innova. The support of Sapienza University by means of the early stage researchers funding is also gratefully acknowledged. H.P. and L.B. acknowledge funding by the European Union (ERC, HYDROGENATE, 101054894)

References

[1] Dreizler, A. et al., “The role of combustion science and technology in low and zero impact energy transformation processes”, *Appl. Energy Combust. Science* 7,100040 (2021).

[2] Matalon, M., “Flame dynamics”, *Proc. Comb. Inst.,* 32(1):57–82, 2009.

[3] Matalon, M., “Intrinsic flame instabilities in premixed and nonpremixed combustion”, *Ann. Rev. Fluid Mech.,* 39(1):163–191, (2007)

[4] Berger, L. et al., “Characteristic patterns of thermodiffusively unstable premixed lean hydrogen flames”, *Proc. Comb. Inst.* 37, 1879–1886 (2019).

[5] Creta, F. et al., “Propagation of premixed flames in the presence of Darrieus–Landau and thermal diffusive instabilities”, *Combust. Flame* 216, 256 (2020)

[6] Lapenna, P.E. et al., “Subgrid modeling of intrinsic instabilities in premixed flame propagation”, *Proc. Comb. Inst.,* 38, (2021).

[7] Lapenna, P.E. et al., “Data-driven subfilter modelling of thermo-diffusively unstable hydrogen–air premixed flames”, *Combust. Theory Model.,* 25, 1064 (2021)

[8] Regele, J.D. et al., “A two-equation model for non-unity Lewis number differential diffusion in lean premixed laminar flames”, *Combust. Flame,* 160(2):240–250, (2013)

[9] Pope, S.B., “Small scales, many species and the manifold challenges of turbulent combustion”, *Proc. Comb. Inst.,* 34(1):1–31, (2013)

[10] Fiorina, B. et al., “A filtered tabulated chemistry model for LES of premixed combustion”, *Combust. Flame* 157, 465 (2010)

[11] Lapenna, P.E. et al., “Large scale effects in weakly turbulent premixed flames”, *Proc. Comb. Inst.,* 37, 1945 (2019)