

Dynamical System Analysis of a Turbulent Premixed Planar Hydrogen Flame in the Corrugated Flamelets Combustion Regime

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Abstract

A direct numerical simulation (DNS) database for hydrogen premixed turbulent flames representative of the corrugated flamelets combustion regime is analysed using the computational singular perturbation (CSP) by incorporating the tangential stretch rate (TSR) approach. It is shown that turbulent flame can be divided roughly into 3 regions: a frozen, explosive, and dissipative state in the direction of the reaction progress. The analysis shows that the flame front can be divided into 2 sub-regions: a diffusion-dominant zone followed by the kinetically controlled zone. In all cases, the dominant processes (reaction and diffusion) are identified. At all time steps, the flame front is successfully tracked as the region where the TSR variable turns positive. Finally, the effect of preferential diffusion is highlighted, where the mixture becomes leaner and richer behind the cusps and the concave parts of the flame fronts, respectively and these features become more pronounced as turbulence increases.

Introduction

Towards development of modern combustion engines, there is growing interest in understanding fundamental characteristics of turbulent premixed flames at high Reynolds (Re) and Karlovitz (Ka) numbers [1,2]. Considering the challenges in realizing such flames in the laboratory and undertaking the quantitative diagnostics of important observables, high fidelity direct numerical simulations (DNS) serve as a valuable approach to analyze the flame characteristics by post-processing the spatially and temporally resolved data. To characterize flame behavior, a rational and unambiguous definition of the flame surface and structure is important. A progress variable, defined as a normalized monotonic reactive scalar variable, is commonly used but this approach faces challenge at high Re/Ka conditions in which the flame structure does not retain the quasi-one-dimensional structure. The problem becomes even more challenging when the upstream reactant mixture has local stratifications. Therefore, a more systematic and universal metric to define and identify the flame is warranted.

The objective of this article is to explore the possibility of utilizing the computational singular perturbation (CSP) analytics, which has been demonstrated as an effective and generalized way to distinguish physical and chemical behavior by automatically identifying the key eigenmodes and their time scales. In recent studies, a derived quantity referred to as the tangential stretching rate (TSR) [3,4] is found to be a comprehensive metric to represent various dynamical characteristics of a reactive-diffusive system. The present study is an initial attempt to utilize this concept in turbulent flame analysis, and to assess the feasibility of using the CSP/TSR tool as a generalized flame analysis.

Laminar Flame

The unstrained laminar solution is used to initialize the DNS calculation. The detailed kinetics mechanism of *Burke et al.* [5] was used and the initial conditions were $T(0)=300\text{K}$, $p(0)=1\text{ atm}$, $\phi=0.7$. For the sake of clarity, the reactions that will be referred to in the later sections are listed in Table 1.

Table 1. The reactions providing significant contribution to the dynamics of the system.

1f:	$\text{H} + \text{O}_2 \Rightarrow \text{O} + \text{OH}$	11f:	$\text{H} + \text{O}_2 (+\text{M}) \Rightarrow \text{HO}_2 (+\text{M})$
2/3f:	$\text{O} + \text{H}_2 \Rightarrow \text{H} + \text{OH}$	13f:	$\text{HO}_2 + \text{H} \Rightarrow 2\text{OH}$
4f:	$\text{H}_2 + \text{OH} \Rightarrow \text{H}_2\text{O} + \text{H}$	15f:	$\text{HO}_2 + \text{OH} \Rightarrow \text{H}_2\text{O} + \text{O}_2$
4b:	$\text{H}_2 + \text{OH} \Leftarrow \text{H}_2\text{O} + \text{H}$		

Following [4], we define $\Omega = \text{Sign}(\omega_\tau) \text{Log}_{10}|\omega_\tau|$ and $\Omega_{\text{pde}} = \text{Sign}(\omega_{\tau,\text{pde}}) \text{Log}_{10}|\omega_{\tau,\text{pde}}|$, so as to appreciate the order of magnitude of both the positive and negative TSR in the same figure. Similarly, the system eigenvalues are defined in the same logarithmic fashion as $\Lambda_i = \text{Sign}(\lambda_i) \text{Log}_{10}|\lambda_i|$.

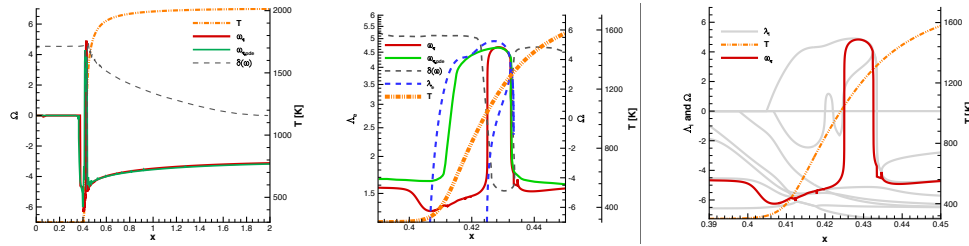


Figure 1. The evolution of Ω_{pde} , Ω , $\log\delta(\omega)$, the eigenvalues Λ_i and the explosive eigenvalues Λ_e of the system, in the case of a laminar H₂/air flame.

In the far upstream region ($x=0-0.37$ mm), the system is in a frozen state, as indicated by the constant values of the species mass fractions, as well as by the negligible chemical source terms (not shown). Fig. 1 shows that the TSR indices, in both the chemical (Ω) and extended version (Ω_{pde}), are zero.

As it is shown in Fig. 2, in the preheat region ($x=0.38 - 0.414$ mm), the largest Participation Indices to TSR mark the chain carrying reaction 4f as the most important process, contributing to approximately 85% of the kinetics-related dynamics. At the same time, the chain termination reaction 11f contributes to the remaining 15%, and increasing.

Fig. 1, in the middle, shows that the flame front is established in a region of $x=0.414-0.435$ mm. This thin region is identified as the area where Ω_{pde} turns positive and can be divided into two subregions based on the dominant role of kinetics or diffusion: (i) in the $x=0.414-0.426$ mm subregion, temperature exhibits the largest increase and $\Omega_{pde}>0$, $\Omega<0$, suggesting that diffusion plays significant role, (ii) in the $x=0.426-0.435$ mm subregion both $\Omega_{pde}>0$ and $\Omega>0$, suggesting that it is kinetics that dominates the dynamics of the system. Fig. 1, on the right, displays the evolution of the system eigenvalues Λ_i as well as the chemical TSR (Ω) in the proximity of the flame front region, highlighting the dissipative scales that are marked by the TSR before and after the chemically-driven subregion.

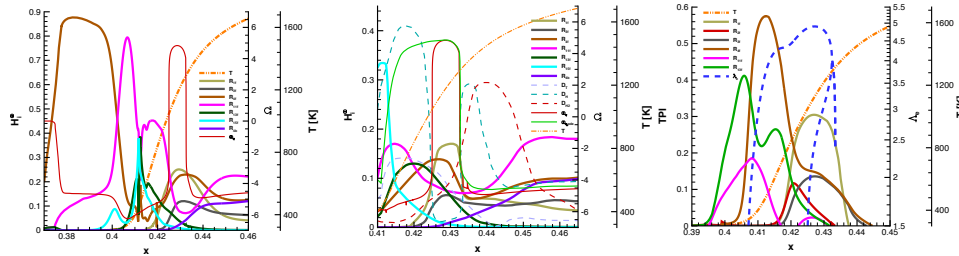


Figure 2. The evolution of the largest TSR Participation Indices (left and middle) along with the largest time scale participation indices (TPI) to Λ_e (right) in the flame front region, in the case of a laminar H_2 /air flame.

Fig. 2 illustrates that in the first subregion of the flame front that is controlled by diffusion, the most significant diffusivities are those from H and temperature. Based on the results provided by the Participation Index to $\omega_{\tau,pde}$ and displayed in Fig. 2, the effect of reactions 11f, 15f and 4f decrease considerably and the prevailing reaction becomes 13f. Additional information about the most significant reactions can be obtained by the results obtained from the time scale participation index (TPI) to the fast explosive timescale. The TPI identifies the chain carrying 4f, the chain branching 13f and the chain terminating 11f as major contributors to the fast explosive timescale. In the second part of the flame front that is dominated by kinetics, the Participation Index to $\omega_{\tau,pde}$ demonstrates that the major contributor to the dynamics of the system is the chain branching 1f; secondary contributions are provided by the chain carrying 4f, the chain branching 3f and the chain termination 11f. All these reactions favor the propensity of the system to explosion, except for reaction 11f, which competes the action of 1f. Additionally, the largest contributor to the explosive timescale at this part of the

process is the chain branching reaction 1f; secondary contribution is provided by 2f/3f and 4f, all of them favoring the explosive nature of the mixture.

In the post-flame front region, Fig. 1 shows that Ω_{pde} becomes negative suggesting that the system turns to a dissipative state. The Participation Indices to TSR reveal that the most important diffusivities are those of H and H₂ and the most important reactions to the dynamics of the system are primarily 11f and secondarily 4f and 4b. The approximately equal contributions of 4f and 4b suggest that these two reactions are in equilibrium. While the effect of the diffusivities of species gradually fades when entering the second part of the downstream region where kinetics prevails, the same set of reactions (i.e., 11f, 4f and 4b) continue to obtain the largest values of participation indices to TSR.

Turbulent Flame

The same approach followed for the laminar case is employed for the dataset generated by means of DNS technique as detailed in [1,2]. The DNS case considered here, which is representative of the corrugated flamelet combustion regime, is characterized by a turbulent Reynolds number $Re_t=227$, a Damkohler number $Da=20.0$ and a Karlovitz number $Ka=0.75$. The domain size is 20 mm x 10 mm x 10 mm and the domain has been discretised by a uniform Cartesian grid of 512 x 256 x 256 cells.

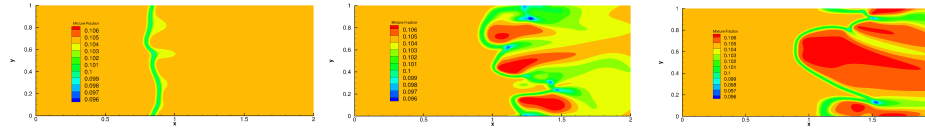


Figure 3. The spatial evolution of the mixture fraction at 3 time steps: $t=2.00E-03$ sec (left), $t=3.00E-03$ sec (middle), $t=5.00E-03$ sec (right).

Fig. 3 shows the mixture fraction as defined by Bilger [6]. At time $t=2.00E-03$ sec, when the flame topology is essentially laminar, the mixture fraction is constant in the entire field with the only exception of the flame front, where the preferential diffusivity of H and H₂ results in a locally leaner mixture in the flame front. At later times, i.e. $t=3.00E-03$ and $t=5.00E-03$, the effects of the 3D nature affect the mixture fraction values in the burnt region, highlighting locally richer and leaner wakes. In particular, the mixture becomes leaner behind the cusps of the flame fronts and richer behind the concave parts of the flame fronts. These features become more pronounced as turbulence increases.

The spatial evolution of Ω_{pde} and $\log\delta(\omega)$ (down) for the 3 time steps is reported in Fig. 4. At all time steps, the flame front is successfully identified as the region where Ω_{pde} turns positive. In the post-flame front region, the system is in a dissipative state, as this is indicated by the negative value of Ω_{pde} . At every time step the distribution of Ω_{pde} , Ω , and $\delta(\omega)$ in the flame front region are in a qualitative agreement with the laminar case, along the entire front. In particular,

moving from the unburnt region to the burnt region, we observe, as shown in Fig. 4, (i) a first subregion where $\Omega < 0$ while $\Omega_{pde} > 0$, indicating a diffusion-driven process; (ii) a second subregion where both $\Omega_{pde} > 0$ and $\Omega_{pde} > 0$, tracking the explosive eigenvalue, in analogy with what shown in Fig. 1 for the laminar case; (iii) a third subregion where both $\Omega < 0$ and $\Omega_{pde} < 0$. In the post-flame region, the role of diffusion requires additional insights, differentiating between the 3 time steps. At $t = 2.00E-03$, the behavior is very similar to the laminar case, where moving farther from the flame front, the two TSR indicators are negative and coincide, meaning that diffusive processes are not relevant, and the system approaches chemical equilibrium on the timescale marked by $\Omega = \Omega_{pde}$. At later times, Ω and Ω_{pde} differ in the post-flame. In particular, the difference is mainly due to Ω_{pde} which highlights the role of preferential diffusion.

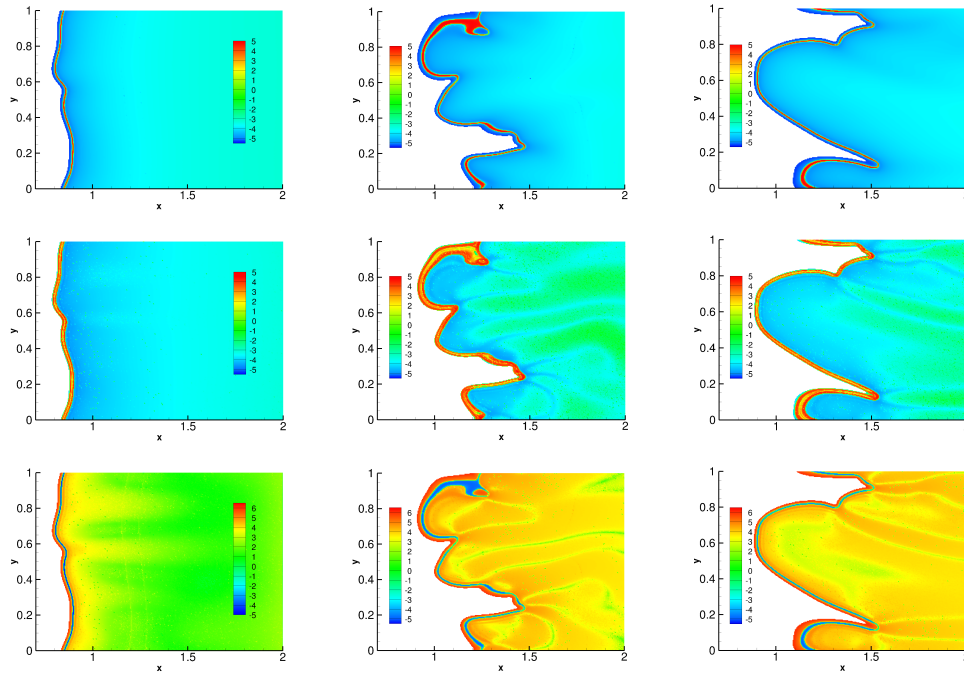


Figure 4. The spatial evolution of Ω (up), Ω_{pde} (middle), and $\delta(\omega)$ (bottom) at 3 time steps: $t = 2.00E-03$ sec (left), $t = 3.00E-03$ sec (middle), $t = 5.00E-03$ sec (right).

Fig. 5 shows the evolution of the TSR Participation Indices of reactions 1f, 4b and 11f and diffusivities of H, H₂ and temperature (down), when $t = 5.00E-03$ sec. Although it is not shown, the chain branching reaction 1f has a dominant role to the explosiveness of the mixture in the flame front region, where kinetics prevails, similarly to what was found in the laminar case. Additionally, the Participation Indices to TSR highlight the importance of reaction 4f and to a less degree 11f, similarly to what was shown in the laminar case. As shown in Fig. 5, in

the downstream region where the system is mostly driven by diffusion, the most significant reactions to the dynamics of the system, which is in dissipative state, are primarily 11f and secondarily 4f and 4b.

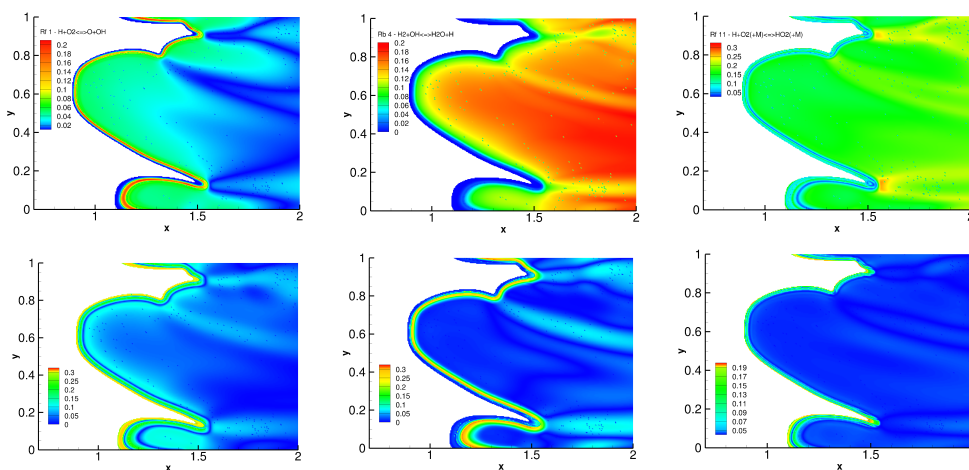


Figure 5. The evolution of the largest TSR Participation Indices of reactions 1f, 4b and 11f (up) and diffusivities of H, H₂ and temperature (down) in the downstream region, when $t=5.0E-03$ sec.

Acknowledgments

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