Explosive Dynamics of Bluff-body-stabilized Lean Premixed Hydrogen Flames at Blow-off

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Abstract

Two-dimensional direct numerical simulation (DNS) databases of bluff-body-stabilized lean hydrogen flames representative of complicated reactive-diffusive system are analysed using the combined approach of computational singular perturbation (CSP) and tangential stretching rate (TSR) to investigate chemical characteristics in blow-off dynamics. To assess the diagnostic approaches in flame and blow-off dynamics, Damköhler number and TSR variables are applied and compared. Four cases are considered in this study showing different flame dynamics such as the steadily stable mode, local extinction by asymmetric vortex shedding, convective blow-off and lean blow-out. DNS data points in positive explosive eigenvalue conditions were subdivided into four different combinations in TSR and extended TSR space and categorized in four distinct characteristic regions, such as kinetically explosive or dissipative and transport-enhanced or dissipative dynamics. The TSR analysis clearly captures the local extinction point in the complicated vortex shedding and allows an improved understanding of the distinct chemistry-

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Preprint submitted to Proceedings of the Combustion Institute 38
transport interactions occurring in convective blow-off and lean blow-out events.

Keywords:
Bluff-body, blow-off, direct numerical simulation, computational singular perturbation, tangential stretching rate

1. Introduction

A bluff-body has been employed as the flame stabilization scheme for many combustion devices such as gas turbines and aviation engines. Although the bluff-body flame holder has a key advantage of generating a hot gas recirculation zone behind it and assist in stable combustion, it also induces flow field and combustion instabilities such as unstable vortex shedding, which can adversely affect the flame stability and lead to blow-off. The understanding of the physical mechanism of flame stabilization and blow-off processes has been one of the critical subjects in premixed combustion systems under highly turbulent conditions. Both experimental [1–4] and numerical [5–9] studies have investigated bluff-body flame stabilization and blow-off dynamics. However, due to the complexities of dynamics behind the bluff-body and many physical and chemical parameters involved, it is difficult to obtain a comprehensive understanding of the flame stabilization and blow-off mechanism.

Shanbhogue et al. [10] reported that lean blow-off behind a bluff-body is a multi-step process starting from local extinction to the ultimate flame shrinking and weakening. They summarized blow-off scaling with characteristic time scales and the corresponding Damköhler number (Da). Our recent
studies [11, 12] investigated stabilization and blow-off mechanisms of bluff-body-stabilized flames and further evaluated the Damköhler number based on various characteristic chemical and flow time scales. The most critical factor to dictate the blow-off limit was found to be the Da based on ignition delay time and lateral fluctuation flow time scale, and proposed ignition Da based on the lateral flow time scale to identify the blow-off criterion. In addition, re-ignition of the local extinction pocket controls the overall blow-off limit, which is consistent with the classical theory by Zukoski and Marble [1]. Considering the complexities in the underlying physical and chemical processes, a systematic and unambiguous statistical analysis to characterize the frequent local quenching and re-ignition events will be highly valuable.

In recent years, computational singular perturbation (CSP) theory has proved to be an elegant tool for such diagnostics, by an automated transformation of the complex chemical systems into a finite number of linearly independent chemical modes comprising the CSP basis vectors and mode amplitudes [13, 14]. The eigenvalue of each chemical mode represents the inverse of the characteristic time scale, and the modes with positive eigenvalues drive the system away from the equilibrium. Both the CSP analysis and the chemically explosive mode analysis (CEMA) [15] have utilized this feature to identify important criticality phenomena - extinction and re-ignition - in $n$-heptane/air and $n$-dodecane/air turbulent reacting flows of DNS datasets [16, 17] and propane/air of LES data [18].

More recently, Valorani et al. introduced the concept of the tangential stretching rate (TSR) [19, 20], which is a single scalar metric defined as a weighted sum of eigenvalues and the corresponding mode amplitudes. The
application to turbulent flames revealed that the TSR index is a more appropriate metric to identify the criticality dynamics rather than using the explosive mode alone [21, 22].

Therefore, the TSR diagnostics may serve as a useful tool to characterize different modes of the flame blow-off which may be some combination of local quenching and re-ignition.

The present study thus aims to assess different diagnostic approaches such as Da and TSRs in blow-off dynamics behind the bluff-body from high-fidelity direct numerical simulation (DNS) data. The main goals of this work are (1) to examine the performance of Da and TSR by applying to DNS data at different conditions, such as steadily stable, local extinction by asymmetric vortex shedding, and total extinction; and thereby (2) to assess if the TSR diagnostics can reveal key differences between the convective blow-off and the lean blow-out phenomena.

2. Methodology

2.1. Configuration and numerical method

The direct numerical simulations (DNS) codes solve the fully compressible multi-species reactive Navier–Stokes equations with a finite difference method of eighth-order accuracy in space and fourth-order in time [23]. A two-dimensional square channel of 10 mm ($H$) with a square-shaped bluff-body stabilizer of 0.5 mm ($D$) was used for a computational domain [11, 12]. The domain size ($H$) was chosen to minimize the confinement effect between the solid walls as the blockage ratio ($D/H$) is 0.05. A test was conducted for different blockage ratios until convergence was reached for the Strouhal num-
ber \( \text{St} = fD/U \) of the vortex shedding for the non-reacting condition [24]. Therefore, the results reported herein are considered those of unconfined flame characteristics.

Hydrogen-air flames are studied employing a detailed kinetics mechanism [25]. Chemical kinetics, thermodynamics, and transport properties were evaluated using CHEMKIN libraries [26], and the mixture-averaged species diffusion model was used [27]. A Cartesian grid with a uniform spacing of \( \Delta x = 10 \mu m \) was chosen based on the resolution requirement for the corresponding reference laminar flame structure by conducting the grid convergence tests with the size of 2.5, 5, 10, and 12.5 \( \mu m \) and the time-step of 10 ns. A typical run with a Cray XC40 cluster (Shaheen II) for time integration up to 10 ms took approximately 8,000 CPU hours. No-slip and adiabatic conditions were applied to the channel walls and bluff-body surfaces. Non-reflecting characteristic boundary conditions were applied to the inflow and outflow boundaries [28, 29]. A fully developed velocity profile with a mean value of inflow velocity \( (U) \) was imposed at the inflow boundary.

2.2. Tangential stretching rate (TSR)

In this subsection, the combined tangential stretching rate (TSR) and computational singular perturbation (CSP) methodology is briefly introduced. Readers may refer to [19, 20] for detailed information.

A reactive system governed by the conservation of species and energy equations is expressed as:

\[
\frac{\partial z}{\partial t} = L(z) + g(z) = \sum_{i=1}^{N+1} a_i(z) h_i(z),
\]

where \( z \) is the state vector that includes the \( N \) species and temperature,
while $g$ and $L$ are the chemical source term and transport operator, respectively. CSP introduces the CSP column basis vectors $a_i$ and related mode amplitudes $h^i$ ($i = 1, ..., N + 1$). Defining $b^i \cdot a_j = \delta^i_j$ with $\delta^i_j$ the Kronecker delta, the amplitude can be represented by $h^i = b^i \cdot (L(z) + g(z))$. To leading order, $a_i$ and $b^i$ can be approximated by the right and left eigenvectors of the Jacobian $J_g$ of the vector field $g(z)$.

Expanding $L$ and $g$ in terms of eigen-modes, the extended version of TSR that considers both chemical reaction and transport, $\omega_{r+d}$, can be introduced as:

$$\omega_{r+d} = \sum_{i=1}^{N+1} W_{i,r+d} \lambda_i,$$

where $\lambda_i$ ($i = 1, ..., N + 1$) is the eigenvalue of the $i$-th mode and the weights $W_i$ are defined as:

$$W_{i,r+d} = \frac{h^i}{L + g} \sum_{k=1}^{N+1} \frac{h^k}{L + g} (a_k \cdot a_i),$$

such that TSR is a weighted sum of all eigenvalues. $L$ and $g$ are the norms of $L$ and $g$, respectively. As such, it is a single scalar metric that properly identifies the true explosive nature of the system since not all explosive modes have sufficiently large amplitude to make a significant impact. The reactive TSR (without the transport) can also be found in case there is no $L$ operator. Thus, the contribution by transport effects are revealed when comparing TSR and extended TSR. It has been shown that a system can be made explosive by the transport process bringing in radical species into the reaction zone [21, 22].

In this study, three different metrics for identifying explosive dynamics are considered: the explosive timescale that is obtained from the conventional
CSP method, TSR ($\Omega_r$) that only considers the chemical reaction without transport, and extended TSR ($\Omega_{r+d}$) that considers both chemical reaction and transport. They are defined as:

$$\Lambda_i = \text{sign}(\lambda_i) \cdot \log_{10}|\lambda_i|,$$

$$\Omega_r = \text{sign}(\omega_r) \cdot \log_{10}|\omega_r|,$$

$$\Omega_{r+d} = \text{sign}(\omega_{r+d}) \cdot \log_{10}|\omega_{r+d}|,$$

and the eigenvalues ($\lambda_i$) less than unity have no meaningful impact on the system. The positive and negative values of $\Lambda$ and $\Omega$ represent the explosive and dissipative behavior. Moreover, all physical time scales are normalized by a nominal time of 1 s so that the magnitudes are non-dimensional.

Table 1: Inflow quantities for lean premixed hydrogen-air with $T_{in} = 300$ K and pressure of 1 atm.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>$\Phi$</th>
<th>$U$ [m/s]</th>
<th>Re$_D$</th>
<th>Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>20</td>
<td>530</td>
<td>Stable</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
<td>75</td>
<td>1990</td>
<td>Local extinction</td>
</tr>
<tr>
<td>3</td>
<td>0.5</td>
<td>85.2</td>
<td>2260</td>
<td>Blow-off</td>
</tr>
<tr>
<td>4</td>
<td>0.194</td>
<td>20</td>
<td>580</td>
<td>Lean blow-out</td>
</tr>
</tbody>
</table>

3. Results and Discussion

The DNS cases under study are summarized in Table 1. Case 1 is the stable flame and serves as the baseline case. Case 2 is at higher inflow velocity and involves local extinction near the flame vortex shedding area.
Cases 3 represents the flame blown off by the large flow velocity and turbulent fluctuations, and Case 4 is a lean blow-out case where the flame quenching occurs due to chemical suppression at low velocity. Cases 1–3 have been reported in the previous study [11], in which the total extinction was observed with the increase of Re. Case 4 is a new case to reproduce a lean blow-out event by decreasing the equivalence ratio starting from Case 1. Cases 3 and 4 are expected to show different extinction dynamics: the blow-off under
highly unstable condition (Case 3) and lean blow-out under the stationary flow condition (Case 4).

To analyze the dynamics of systems, four different diagnostic approaches are used, including Da, \( \Lambda_e \), \( \Omega_r \), and \( \Omega_{r+d} \). Da is computed from the species conservation equations (ratio of reaction and diffusive terms) by defining a progress variable \( (c) \) in terms of three species mass fractions (HO\(_2\), OH, and...
H$_2$O), which monotonically increases from $c = 0$ at the unburned gas side to $c = 1$ at the fully burned state. Da is computed for the progress variable in the range 0.05–0.95.

3.1. Overall Characteristics

Figure 1 displays representative snapshots of each case where the isocontour of water mass fraction at 50 % of the equilibrium value is also overlaid on each figure, showing the typical shape of the flame topology as well as the local extinction point (an open circle) at $x = 5.02$ mm at the center of the y-axis for Case 2. The corresponding distributions of the diagnostics metrics, Da, explosive eigenvalue ($\Lambda_e$), TSR ($\Omega_r$), and extended TSR ($\Omega_{r+d}$) are also sequentially shown from Fig. 2 to Fig. 5. From Fig. 1 to 5 the y-axis shows the range $y = [3 : 7]$ mm. Note that the scale in the color map for Da is different from others since Da has only a positive value.

Figure 2 shows the distinct pictures portrayed by different metrics. Da shows the sharp reaction zones (red) and the intermediate range (green) in the product region. $\Lambda_e$ shows the region of explosive dynamics as a broader layer around the main reaction zone. In contrast, $\Omega_r$ demarcates a thin layer of chemically explosive region which is rather on the back side of the positive $\Lambda_e$ layer, implying that not all $\Lambda_e > 0$ region represent explosive dynamics. Finally, the extended TSR, $\Omega_{r+d}$ shows yet another explosive layer just in front of the $\Omega_r > 0$ region, and this region is characterized as a region of explosive dynamics due to transport. As such, the combined $\Omega_r$ and $\Omega_{r+d}$ diagnostics would properly identify the correct explosive zones and their underlying mechanisms.

The application of the same diagnostics to the local extinction case (Case
2) in Fig. 3 shows more distinct and complicated images. At the location identified as a local extinction point in Fig. 1 (denoted by an open circle) based on a progress variable of normalized water mass fraction [11], obviously Da indicates a small number (black). However, \( \Lambda_e \) and \( \Omega_r \) do not show any clear sign of the local extinction, implying that the extinction event is not distinguishable from a pure kinetics perspective. On the other hand, \( \Omega_{r+d} \) marks this location as a negative region, implying that the local extinction was caused by the dissipative transport due to the vortex shedding.

![Isocontours](image)

**Figure 4:** Isocontours of Da, \( \Lambda_e \), \( \Omega_r \), and \( \Omega_{r+d} \) for case 3.

Figures 4 and 5 show the results for the convective blow-off (case 3) and lean blow-out (case 4), respectively. For both cases, the Da distribution closely follows the isocontours shown in Fig. 1, visualizing the main flame regions. In contrast, \( \Lambda_e \) does not show any dissipative state in Fig. 4, while the lean blow-out in Fig. 5 appears as if non-reacting asymmetric vortex shedding occurs at the end of attached flames. The positive \( \Omega_r \) areas are clearly reduced in both cases 3 and 4, and comparison with \( \Omega_{r+d} \) helps identify
the role of transport in the quenching process.

Based on these overall qualitative observations, a more quantitative and statistical assessment of different diagnostics is performed in the following section.

3.2. TSR versus Da Analysis

The local characteristic Da has commonly been used to identify the flame extinction and re-ignition. Since the definition of Da requires a choice of specific species presumed to be a key marker, it may lose validity in general turbulent flame conditions. To assess the validity of the newly proposed metrics, the relation between (a) $\Lambda_e$, (b) $\Omega_r$, and (c) $\Omega_{r+d}$ and Da are shown as a scatter plot in Fig. 6 and Fig. 7. Since the eigenvalues ($\lambda_i$) less than unity have no meaningful impact on the system, all eigenvalues less than unity are not shown. Therefore, positive and negative values of $\Omega$ represent the explosive and dissipative behaviors in explosive eigenvalues only.

For the stable flame (case 1) in Fig. 6, the solution states of $\Lambda_e$ and $\Omega_{r+d}$
span the range of Da from 0 to 5. It is first seen that the $\Lambda_e$ assumes large positive values over a broad conditions at Da. However, $\Omega_r$ for the same data points shows that part of these locations has dissipative dynamics, as denoted by the green colored data points. As such the overall behavior resembles a typical S-curve response. Therefore, while all the data points are considered explosive by the $\Lambda_e$ metric, comparison of $\Omega_r$ and $\Omega_{r+d}$ distinguishes these points to be in chemically-driven (red) and transport-driven (green) explosive dynamics.

For case 2 (Fig. 7) in the presence of some partial quenching, the solution state is more concentrated in the lower Da (less than 2) zone. Furthermore, the data points with negative $\Omega_{r+d}$ originate partly from positive and negative
\(\Omega_r > 0\) and \(\Omega_{r+d} > 0\)

\(\Omega_r < 0\) and \(\Omega_{r+d} > 0\)

\(\Omega_r < 0\) and \(\Omega_{r+d} < 0\)

\(\Omega_r > 0\) and \(\Omega_{r+d} < 0\)

Figure 7: Scatter plots of (a) \(\Lambda_e\), (b) \(\Omega_r\), and (c) \(\Omega_{r+d}\) against Da and (d) \(\Omega_{r+d}\) against \(\Omega_r\) for case 2.

\(\Omega_r\) conditions, denoted as orange and grey colors, respectively. Therefore, the locations of positive \(\Lambda_e\) conditions are further subdivided into four different combinations in \(\Omega_r\) and \(\Omega_{r+d}\), and characterized as:

1. (Q1) Reactive region: \(\Omega_r > 0\) and \(\Omega_{r+d} > 0\).
2. (Q2) Preheat region: \(\Omega_r < 0\) and \(\Omega_{r+d} > 0\).
3. (Q3) Dissipative region: \(\Omega_r < 0\) and \(\Omega_{r+d} < 0\).
4. (Q4) Local extinction region: \(\Omega_r > 0\) and \(\Omega_{r+d} < 0\).

These regions occupy Quadrant 1 through 4, in the \(\Omega_{r+d}\) versus \(\Omega_r\) diagram shown in Fig. 6(d) and Fig. 7(d). Quadrant 1 and 3 are kinetically driven as \(\omega_r \approx \omega_{r+d}\) so that \(\Omega_r\) dictates the nature (either explosive or dissipative) and the contribution of transport is negligible. In Quadrant 2 and 4,
the contribution of transport overrides against the $\Omega_r$ characteristics in the net explosive/dissipative characteristics.

With the above criteria, it is possible to backtrack key features in different locations such as the exact local extinction points. The ultimate explosive dynamics in the local points is determined by $\Omega_{r+d}$. The states associated with the local extinction region (Quadrant 4) appear in the lower Da zone (values between 0 and 2) in Fig. 7(c). With the information of each region based on $\Omega_r$ and $\Omega_{r+d}$, the correct local dynamics are captured, which was not possible with either Da or $\Lambda_e$ alone.

Figure 8: Conditioned $\Omega_r$ and $\Omega_{r+d}$ of the DNS data points on the physical space for (a, b) case 2, (c, d) case 3, and (e, f) case 4.
3.3. TSR Analysis of Extinction

To identify the actual locations of the regions corresponding to Q1–Q4, the same color map is overlaid on the physical space in Fig. 8 for cases 2, 3, and 4. Figure 8(a) depicts the situation when transport enhances the explosive characteristics (green). On the other hand, Fig. 8(b) indicates the situation when transport drives the system to dissipative states (orange). It is also noted that both of the explosive locations (green and red) correspond well with the heat release rate shown in Fig. 1 and the occasional local extinction points are shown in negative $\Omega_{r+d}$ conditions (grey and orange) along the reactive fronts. The transport-driven explosiveness in Fig. 8(a) is observed around the local extinction place that shows the likelihood of re-ignition [11, 12].

A similar analysis is now performed for cases 3 and 4 and the results are shown in Fig. 8(c)/(d) and (e)/(f), respectively.

For Case 3 of convective blow-off, although transport supports the ex-
plosive characteristics (green), some of these regions enhance dissipative effects (orange). In particular, an important location is the recirculation zone (around $x = [2.5, 4.0] \text{ mm}$) where the flame is associated with a more chemically dissipative state (grey points in Fig. 8(c)). At the same location, there is more transport-driven dissipation (orange) in Fig. 8(d). This suggests that the extinction is caused by larger effects of transport. In contrast, for lean blow-out (case 4) shown in Fig. 8(f), the area of the reactive zone (mainly $x = [3.5, 4.5] \text{ mm}$) is very small. Consequently, even if transport supports the explosiveness (green), the flame is chemically not sustainable (i.e. red points are much reduced). In summary, the convective blow-off is characterized by the intense chemical reactions suppressed by transport-driven dissipation (orange), while the lean blow-out is driven by the overall chemical suppression regardless of the transport effect.

Figure 9 summarizes the fraction of data points in each quadrant of the TSR map for all cases. Both cases 1 and 2 clearly show that both kinetically explosive state (Q1) and transport enhanced kinetic explosiveness (Q2) are dominant. In the local extinction case (case 2), dissipative states by kinetic and transport (Q3 and Q4) appear, while case 1 has no presence of Q4. The dominance of chemical explosiveness (Q1) is decreased in case 3, while dissipative state (Q3) is increased. Although the transport-enhanced explosiveness (Q2) becomes dominant for cases 3 and 4, their relative fraction is found to be decreased as approaching the convective blow-off (from case 1 to 3) as well as at the lean blow-out (case 4). Again, the main distinction between cases 3 and 4 is seen as the lean blow-out (case 4) exhibits a drastically low level of chemically and transport-driven explosive dynamics.
(Q1), despite the enhanced transport-driven explosiveness (Q2) such that no re-ignition and recovery are possible.

It must be stated that both cases 3 and 4 have frequent extinction and re-ignition events in rapid transients, such that the analysis of a single instantaneous solution field may not reveal the detailed temporal dynamics. Such an analysis will be conducted and reported in future work.

4. Conclusions

Tangential stretching rate (TSR) analysis was carried out using two-dimensional high fidelity numerical simulations of bluff-body-stabilized lean premixed hydrogen flames in a square channel to examine the capability of different diagnostics. The total of four cases were considered in this study showing different flame dynamics, such as the steadily stable, local extinction by asymmetric vortex shedding, convective blow-off, and lean blow-out conditions. In particular, two different extinction cases of convective blow-off and lean blow-out were analyzed based on various analytical diagnostics.

Comparisons of different diagnostic variables such as Damköhler number (Da), explosive eigenvalue (Λe), TSR (Ωr), and extended TSR (Ωr+d) were attempted to identify the key features of the flames and contribution of kinetics and transport in the dynamics. The solution points were categorized in a single TSR map of four quadrants based on zero-crossing of Ωr and Ωr+d such as kinetically explosive or dissipative and transport-enhanced or dissipated dynamics. Mapping the Ωr and Ωr+d characteristics onto the spatial locations in the physical space allowed an improved understanding about the distinct chemistry-transport interactions occurring in convective blow-off and
lean blow-out events.

Acknowledgments

This work was sponsored by King Abdullah University of Science and Technology (KAUST). Computational resources were provided by the KAUST Supercomputing Laboratory (KSL). The authors would like to thank Professor Mauro Valorani and his group at Sapienza University of Rome for providing the CSP analysis tools.

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