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Flamelet Regime Characterization for Turbulent Combustion Simulations

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Abstract

Regime characterization has been shown to be an insightful technique in the study of turbulent combustion, providing useful information about the relation between fundamental combustion modes and physical scales that require consideration. Regime diagrams can provide guidance to the appropriate utilization of combustion models, which is critical for the accuracy of numerical simulations of turbulent reacting flows. In the present study, a flamelet regime diagram is developed to assess the applicability of various diffusion flamelet models with respect to the local grid resolution and underlying flow/flame structure. The flamelet regime parameter is defined such that it can be unambiguously determined with fully resolved data, as in the case of direct numerical simulations (DNS), and reasonably estimated by resolved, filtered information of large-eddy simulations (LES). To this end, the flamelet regime diagram is studied through an *a priori* analysis of a DNS dataset of a turbulent lifted hydrogen jet flame in a heated coflow. Findings from this analysis verify the length-scale arguments that are based on the concepts of inner-reaction zone thickness and dissipation element, on which the regime diagram is constructed. In addition, the relevance of the regime diagram to the numerical grid size enables its employment as a guiding tool for model selection in combustion LES.

Keywords: Flamelet modeling, Diffusion flame, Regime characterization, Direct numerical simulation

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1. Introduction

Among the many studies of turbulent flames, the characterization of the combustion mode of a flame remains a topic of interest. For instance, using characteristic length- and velocity-scales of a combustion system, Mellor and Ferguson [1] mapped out regions that correspond to different applications, including internal combustion engines, gas-turbine combustors, and fires. From this diagram, practical engine configurations and fire are separated by the order of their sizes, speeds, and sensitivity to buoyancy. Such relations between a flame-type and its properties demonstrate one of the useful aspects of regime diagrams.

Another type of regime diagrams was developed by Borghi [2], Peters [3], and Williams [4]. Using length- and velocity-scale ratios, as in the case of Borghi and Peters, or non-dimensional Reynolds and Damköhler numbers, as in the study of Williams, these regime diagrams consider a time-scale that is relevant to combustion, in contrast to that by Mellor and Ferguson [1], which contains only information of the system level. Specifically, the Borghi-Peters (and Williams) diagram delineates regions such as the broken (distributed) reaction and low-Karlovitz (high-Damköhler) number zones. The regime diagram also identifies a thin-reaction (broken-flamelet) zone, in which the smallest turbulent structures can penetrate only the flame layer, but not the inner reaction layer.

Recognizing the state relation between mixture fraction and thermochemical variables, Peters [5] constructed a regime diagram that considers the fluctuation of mixture fraction and mean scalar dissipation rate at stoichiometric condition. For a methane-air jet flame, Peters' diagram is able to relate the flame properties at different regions (e.g. lift-off and equilibrium) to the effects of turbulence on the mixture fraction field.

In some instances, researchers are interested in diagrams that relate their methodologies to the various flame regimes. One example was introduced by Pitsch and Duchamp de Lageneste [6], which replaced the integral turbulent scales of Peters diagram [5] by the numerical subgrid-scales (SGS) of large-eddy simulations (LES). In doing so, along with the utilization of the filter-width independent Karlovitz number, they identified limits of various forms of the G-equation model [4, 7, 8] with respect to the filter size of LES of turbulent premixed combustion. These results provided a consistency requirement for turbulent premixed combustion models, stating that the filter width cannot affect the underlying combustion mode, namely the wrinkled/corrugated flamelets, thin-reaction zone, and broken reaction-zone regimes.

Essentially, the variety in regime diagrams illustrates that the parameterization of turbulent flames in terms of only two variables, although insightful, can be insufficient for the overall picture. For example, Williams [9] suggested that the scalar dissipation rate can be included as a third coordinate to the Williams diagram [4]. Düsing *et al.* [10] extended the Borghi-Peters diagram with a third dimension that spans the ordinate of the diagram by Pitsch and Duchamp de Lageneste, identifying as many as 26 unique regions for the classification of premixed combustion models. While feasible, this approach increases the spatial complexity in the evaluation, which can be intractable and hence less desirable. As a result, researchers continued to develop distinct regime diagrams, each focusing on a certain aspects of turbulent flames. Accordingly, even Düsing *et al.* returned their discussions to a two-dimensional representation of their extended Borghi-Peters diagram.

Due to recent advancements in computational capabilities, direct numerical simulation (DNS) of turbulent combustion is becoming more relevant to practical combustion systems, thus establishing itself as a valuable tool to complement combustion experiments and theories [11]. Consequently, the systematic extraction of flame regimes from DNS data gains attention from the fundamental flame-index [12] to comprehensive metrics, such as combustion model compliance indicators [13]. Using DNS of a turbulent jet flame, Scholtissek *et al.* [14] developed a regime diagram that delineates limits where the one-dimensional flamelet formulation is inadequate due to the presence of differential diffusion and multi-dimensional effects. Their findings confirmed that the contributions from higher-order expansion terms, which are omitted by the classical flamelet model, are typically dependent on the curvature of the mixture-fraction field and flame thickness, and hence should be considered in the general case.

The objective of the current study is to investigate the applicability of different diffusion flamelet formulations [15] with respect to the LES filter-width. Through this study, a quantitative tool for the suitability of a chosen diffusion flamelet model will be provided, alleviating the ambiguity of conventional *a posteriori* assessments of the model's compatibility to flame conditions. To this end, a flamelet regime diagram that

compares the effective dimensionality of flamelets against the LES filter-width is constructed. Applying length-scale arguments based on concepts of inner-reaction zone thickness [16] and dissipation element [17], the proposed regime diagram is shown to relate to the Karlovitz number for non-premixed flames. Contrary to previous regime analyses, emphasis of this study is placed particularly on: (i) the unambiguous definition of the diagram parameters, which can be precisely evaluated at every instant so that statistical analysis is not required; and (ii) the depiction of the diagram using only resolved information in the case of LES. Furthermore, because of its relevance to the LES filter-width, the current regime diagram is shown to be useful in guiding the model selection procedure in LES.

The outline of this work is as follows. In the next section, the derivation of the regime diagram and its approximation with LES filtered data are discussed. Subsequently, the DNS dataset, generated from the work of Yoo *et al.* [18], is described, followed by the discussion of the results from the *a priori* regime analyses in Sec. 4. Finally, conclusions are drawn.

2. Mathematical Formulations

In this section, the underlying mathematics of the flamelet regime diagram is described, introducing the regime parameter derivation and approximations in terms of filtered information. In addition, a length-scale analysis is performed using concepts that are relevant to dissipation element theory [17] and reaction-zone thickness [16].

2.1. Regime Parameter Derivation

The species transport equation for reacting flows is given by:

$$\frac{\partial Y_\alpha}{\partial t} + u_i \frac{\partial Y_\alpha}{\partial x_i} = -\frac{1}{\rho} \frac{\partial}{\partial x_i} (\rho v_{\alpha,i} Y_\alpha) + \dot{\omega}_\alpha, \quad (1)$$

where Y_α is the mass-fraction, u_i is the flow velocity aligned in the i th direction, ρ is the mixture density, $\dot{\omega}_\alpha$ is the reaction-rate, and the subscripts α and i denote, respectively, specie α and index-notation. The diffusive velocity of the N_s species, $v_{\alpha,i}$, is given by [19]:

$$\begin{aligned} v_{\alpha,i} &= v_{\alpha,i}^F + v_i^C \\ &= -\frac{D_\alpha}{Y_\alpha} \left(\frac{\partial Y_\alpha}{\partial x_i} + \frac{Y_\alpha}{W} \frac{\partial W}{\partial x_i} \right) + \sum_{\beta=1}^{N_s} \left[D_\beta \left(\frac{\partial Y_\beta}{\partial x_i} + \frac{Y_\beta}{W} \frac{\partial W}{\partial x_i} \right) \right], \end{aligned} \quad (2)$$

where D_α is the diffusivity of specie α and W is the mixture molecular weight. The superscripts F and C refer to Fick's law of diffusion and correction-velocity for mass conservation, respectively, and the latter equation implies the implementation of Curtis-Hirschfelder approximation for species diffusion velocities [20].

In accordance with Pitsch & Peters [21], the one-dimensional transport equations of species and temperature are exactly represented by the corresponding flamelet equations. Previous studies [14, 22] have indicated that the flamelet equations in multi-dimensional space are satisfied by quasi-one-dimensional flamelets, which are essentially mixture-fraction gradient trajectories and coordinate-invariant [23]. Hence, the multi-dimensional flamelet equations can be interpreted as the counterparts of the locally rotated Eqs. (1) on each point of a flamelet, such that:

$$x_i \rightarrow X_j, \quad u_i \rightarrow U_j, \quad v_{\alpha,i} \rightarrow V_{\alpha,j}, \quad (3a)$$

$$\frac{\partial Z}{\partial X_j} = \left[\left| \frac{\partial Z}{\partial x_i} \right|, 0, 0 \right]^T, \quad (3b)$$

$$\begin{aligned} \frac{\partial}{\partial x_i} \rightarrow \frac{\partial}{\partial X_j} &= \underbrace{\left[\frac{1}{|\nabla Z|} \frac{\partial Z}{\partial x_i} \frac{\partial}{\partial x_i}, 0, 0 \right]^T}_{\text{projection } \parallel \nabla Z} + \underbrace{\left[0, \frac{\partial}{\partial X_2}, \frac{\partial}{\partial X_3} \right]^T}_{\text{projection } \perp \nabla Z} \\ &= \left(\frac{1}{|\nabla Z|^2} \frac{\partial Z}{\partial X_j} \right) \frac{\partial Z}{\partial x_i} \frac{\partial}{\partial x_i} + \nabla_j^\perp. \end{aligned} \quad (3c)$$

Equation (3b) implies that the X_1 -direction of the rotated frame with respect to the Cartesian frame is aligned with the mixture-fraction gradient described by the Cartesian x_i -coordinates. Correspondingly, the coordinates in orthogonal directions to X_1 are denoted by $X_{j \neq 1}$, for which the derivative vector, $[0, \partial/\partial X_{j \neq 1}]^T$, is represented by the shorthand, $\nabla_j^\perp$. Note that details on the construction of a three-dimensional X_j coordinate system can be found in Refs. [15] and [23].

Figure 1: Local frame rotation for the contribution of diffusion in the flame-aligned reference frame. The blank and shaded regions are occupied by the fuel and oxidizer, respectively, which are separated by the stoichiometric mixture fraction, Z_{st} . The x_i - and X_j -coordinates refer to the Cartesian and rotated frame, respectively.

The transport equation (1) can then be rewritten in the rotated frame coordinates, X_j :

$$\frac{\partial Y_\alpha}{\partial t} + U_j \frac{\partial Y_\alpha}{\partial X_j} = -\frac{1}{\rho} \frac{\partial}{\partial X_j} (\rho V_{\alpha,j} Y_\alpha) + \dot{\omega}_\alpha, \quad (4)$$

In this rotated frame, the definition of the mixture fraction by Pitsch & Peters [21] obeys the transport

equation:

$$\frac{\partial Z}{\partial t} + U_1 \frac{\partial Z}{\partial X_1} = \frac{1}{\rho} \frac{\partial}{\partial X_j} \left(\rho D_Z \frac{\partial Z}{\partial X_j} \right), \quad (5)$$

where the rotation condition of Eq. (3b) has been implied.

Using Eqs. (4) and (5) and recognizing that [22]:

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z} - (u_i - (u_k \hat{n}_k) \hat{n}_i) \frac{\partial}{\partial x_i} \quad (6a)$$

$$= \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z} - \sum_{j=2}^3 \left(U_j \frac{\partial}{\partial X_j} \right), \quad (6b)$$

where $\hat{n}_i = \nabla Z / |\nabla Z|$, and from [14] that:

$$\frac{\partial}{\partial Z} = \frac{\hat{n}_i}{|\nabla Z|} \frac{\partial}{\partial x_i} = \frac{1}{|\nabla Z|} \frac{\partial}{\partial X_1}, \quad (7)$$

the multi-dimensional species flamelet equations can be derived as:

$$\begin{aligned} \frac{\partial Y_\alpha}{\partial \tau} = & \underbrace{\frac{\chi_Z}{2\text{Le}_\alpha} \frac{\partial^2 Y_\alpha}{\partial Z^2}}_{\mathcal{J}_{\alpha,1}^{YZ}} + \omega_\alpha \\ & + \underbrace{\frac{1}{\rho} \left[\frac{\rho \chi_Z}{2} \frac{\partial}{\partial Z} \left(\frac{1}{\text{Le}_\alpha} \right) + \frac{1}{4} \left(\frac{1}{\text{Le}_\alpha} - 1 \right) \left(\frac{\partial \rho \chi_Z}{\partial Z} + \frac{\chi_Z}{D_Z} \frac{\partial \rho D_Z}{\partial Z} \right) \right]}_{\mathcal{J}_{\alpha,2}^{YZ}} \frac{\partial Y_\alpha}{\partial Z} \\ & + \underbrace{\frac{1}{\rho} \frac{\partial}{\partial X_j} \left(\frac{\rho D_Z}{\text{Le}_\alpha} \nabla_j^\perp Y_\alpha \right)}_{\mathcal{J}_{\alpha}^{Y\kappa}} - \underbrace{\left(\frac{1}{\text{Le}_\alpha} - 1 \right) \sqrt{\frac{\chi_Z D_Z}{2}} \kappa_Z}_{\mathcal{J}_{\alpha}^{Y\perp}} \frac{\partial Y_\alpha}{\partial Z} \\ & + \underbrace{\frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\rho \left(-V_{\alpha,j} Y_\alpha - D_\alpha \frac{\partial Y_\alpha}{\partial X_j} \right) \right]}_{\mathcal{J}_{\alpha,1}^{WZ} + \mathcal{J}_{\alpha,2}^{WZ} + \mathcal{J}_{\alpha}^{CZ} + \mathcal{J}_{\alpha}^{W\kappa} + \mathcal{J}_{\alpha}^{W\perp} + \mathcal{J}_{\alpha}^{C\perp}}, \end{aligned} \quad (8)$$

where $\text{Le}_\alpha = D_Z / D_\alpha$ is the Lewis number of specie α . In Eq. (8), the scalar dissipation rate is

$$\chi_Z = 2D_Z |\nabla Z|^2 = 2D_Z \left(\frac{\partial Z}{\partial X_1} \right)^2, \quad (9)$$

and the curvature of the mixture-fraction field is

$$\kappa_Z = -\frac{\partial}{\partial x_i} (\hat{n}_i) = \frac{-1}{|\nabla Z|} \frac{\partial}{\partial X_j} (\nabla_j^\perp Z). \quad (10)$$

Since the frame rotation is locally implemented, the X_2 and X_3 components of the mixture-fraction gradient may not be zero everywhere and thus have to be retained in Eq. (10). For reference, the derivations of Eqs. (8) and (10) are given in [Appendix A](#).

In Eq. (8), the terms containing the $\partial_Z(\cdot)$ derivatives, hereafter defined as the flame-orthogonal terms, relate to the gradients in only the X_1 -direction and correspond exactly to the full one-dimensional species

flamelet equation by Pitsch & Peters [21]. In contrast, the $\nabla_j^\perp(\cdot)$ terms, defined as the flame-aligned terms, are given by the divergence of gradients in only the X_2 - and X_3 -directions and account for the multi-dimensional flamelet effects introduced by Scholtissek *et al.* [14]. Hence, the derivation of Eq. (8) shows that: (i) the transport equations in both the Cartesian and rotated frames will transform to the same flamelet equations; and (ii) the flamelet transformation is essentially a local decomposition of effects in the flame-aligned and flame-orthogonal directions, as demonstrated by the frame rotation.

Using Eq. (8), we can define a flamelet regime parameter that delineates regions within a turbulent flow where the conventional Pitsch-Peters flamelet formulation [21] applies, differentiating from those where the multi-dimensional flamelet concept [14] requires consideration. This parameter is given as:

$$\psi_\alpha = \frac{\sum_{j=2}^3 -\frac{\partial}{\partial X_j} [\rho V_{\alpha,j} Y_\alpha] - \frac{\partial}{\partial X_j} \left[\rho D_Z \frac{\partial Z}{\partial X_j} \right] \frac{\partial Y_\alpha}{\partial Z}}{-\frac{\partial}{\partial X_1} [\rho V_{\alpha,1} Y_\alpha] - \frac{\partial}{\partial X_1} \left[\rho D_Z \frac{\partial Z}{\partial X_1} \right] \frac{\partial Y_\alpha}{\partial Z}} \quad (11a)$$

$$= \frac{\mathcal{J}_\alpha^{Y\perp} + \mathcal{J}_\alpha^{W\perp} + \mathcal{J}_\alpha^{Y\kappa} + \mathcal{J}_\alpha^{W\kappa} + \mathcal{J}_\alpha^{C\perp}}{\mathcal{J}_{\alpha,1}^{YZ} + \mathcal{J}_{\alpha,1}^{WZ} + \mathcal{J}_{\alpha,2}^{YZ} + \mathcal{J}_{\alpha,2}^{WZ} + \mathcal{J}_\alpha^{CZ}}, \quad (11b)$$

where the numerator and denominator transform to the flame-aligned (i.e. curvature and multi-dimensional effects) and flame-orthogonal (i.e. classical flamelet diffusion effects) terms, respectively.

Therefore, the ratio in Eq. (11) represents the competition between diffusion in the flame-aligned direction to that in the flame-orthogonal direction, essentially evaluating the multi-dimensional diffusion relative to the quasi one-dimensional diffusion along a flamelet. The different types of diffusion are depicted in Fig. 2, where the multi-dimensional diffusion (due to flame propagation and mixture-fraction curvature) is indicated by solid arrows and the flamelet diffusion is denoted by dashed arrows.

The compactness of Eq. (11) demonstrates that the local frame rotation is a useful methodology in the evaluation of flamelets. More importantly, the local frame rotation allows for the evaluation of diffusion in the flame-aligned and flame-orthogonal directions without the need to evaluate second derivatives in mixture-fraction space, which tends to introduce numerical noise in the flamelet analysis.

2.2. Length-Scale Analysis for Regime Diagram

The flamelet regime parameter of Eq. (11), ψ_α , has been identified as the ratio of diffusion in the flame-aligned direction to that in the flame-orthogonal direction. Similar to Ref. [14], this ratio can be approximated through a scaling argument:

$$\psi_\alpha \sim \frac{\Delta Y_\alpha^\perp}{(l^\perp)^2} \frac{(l^Z)^2}{\Delta Y_\alpha^Z} = (\Delta Z)_R \left(\frac{l^Z}{l^\perp} \right)^2, \quad (12)$$

where $(\Delta Z)_R$ is the reaction-zone thickness in mixture-fraction space [16], and l denotes the characteristic length-scale in flamelet related directions, which are indicated by the superscripts $\perp$ and Z as the directions

Figure 2: Two types of diffusion around a flamelet (solid straight line). The blank and shaded regions are occupied by the fuel and oxidizer, respectively, which are separated by the stoichiometric mixture fraction, Z_{st} (solid curve). The contour lines indicate the flame. The multi-dimensional and quasi one-dimensional flamelet diffusion effects are denoted by solid and dashed arrows, respectively.

orthogonal (flame-aligned) and parallel (flame-orthogonal) to the mixture-fraction gradient, respectively. Note that Eq. (12) is scaled with the square of a length-scale because it is relevant to diffusion effects. The $(\Delta Z)_R$ is typically small in the mixture-fraction space, and hence a relevant scaling variable for the expectedly small ratio of $\Delta Y_\alpha^\perp / \Delta Y_\alpha^Z$ in diffusion flames [14].

In their study, Scholtissek *et al.* [14] attributed the higher-order flamelet effects to the corrugation of the mixture-fraction field, thereby scaling the orthogonal length-scale $l^\perp$ by the reciprocal of the mixture-fraction curvature. However, due to the multi-dimensionality of turbulence, the interaction of flamelets should be feasible regardless of the corrugation intensity of the mixture-fraction field. Hence, a more appropriate definition of $l^\perp$ will be based on the concept of the dissipation element [17], which is a notional turbulent structure that is characterized by the Kolmogorov length-scale, η_K , for a practical range of Taylor-Reynolds number up to $\mathcal{O}(10^2)$. For the representative flame-orthogonal length-scale, l^Z , of Eq. (12), we will follow the arguments presented in Ref. [14] and scale the term by the reaction-zone thickness, δ_R , thus giving:

$$l^Z \sim \delta_R, \quad l^\perp \sim \eta_K, \quad (13a)$$

$$\log[\psi_\alpha] = -2 \log\left[\frac{\Delta}{\delta_R}\right] + \log\left[2Z_{st} \left(\frac{\Delta}{\eta_K}\right)^2\right], \quad (13b)$$

where the symbol Δ indicates the grid spacing, and Z_{st} is the stoichiometric mixture fraction. For LES with Δ of the order of the integral length-scale, Λ , the ratio Δ/η_K can be written as $\text{Re}_\Lambda^{3/4}$, based on Kolmogorov's

turbulence theory.

The term $(2Z_{st})$ in Eq. (13b) arises from the estimation of $(\Delta Z)_R$ using Peters' approximation for the diffusion flame thickness in mixture-fraction space, $(\Delta Z)_F \approx 2Z_{st}$ [24]. Note that such estimation should over-predict $(\Delta Z)_R$, since, in accordance with Peters [5],

$$(\Delta Z)_R = \epsilon(\Delta Z)_F, \quad \text{with } \epsilon < 1, \quad (14)$$

resulting in a more conservative condition for the order-of-magnitude estimate of η_K for a given ψ_α .

A point that is noteworthy from the length-scale perspective of Eqs. (12) and (13b) is its generality among species (i.e. lack of dependence on α on the right-hand-side). Therefore, one can expect that the regime parameter will remain of similar leading order regardless of species α , a trend that is confirmed in the later section of this work.

From Eq. (13b), different regimes can be demarcated, as illustrated in Fig. 3, where Δ/δ_R and ψ_α span the x - and y -axis, respectively. The broadest categorization is separated by the abscissa. The left and right quadrants above this line (i.e. $\psi_\alpha > 1$) are characterized by significant flamelet interaction, hence invalidating the isolated flamelet model that considers only diffusion along a flamelet. For this reason, we will refer to this region as the *Multi-Dimensional Flamelet Regime* [14]. Below the abscissa (i.e. $\psi_\alpha \leq 1$), a region, which is defined by:

$$\psi_\alpha/2Z_{st} = (\delta_R/\eta_K)^2 = \text{Ka}_K \leq 1,$$

can be extracted. A flame satisfying this condition will have a reaction zone that is thinner than the smallest turbulent eddy, which, in accordance with Peters [5], is the criterion for the validity of the isolated flamelet theory. Hence, we will refer to this zone as the *Peters' Regime*. The line $\text{Ka}_K = 100$ is the validity limit for flamelet theory [5], which will be used later to assess the applicability of the flamelet formulation.

The area distinguished by the limits $2Z_{st} \leq \psi_\alpha \leq 1$ ($\text{Ka}_K = 1$ and the abscissa, respectively) can be interpreted as a transition region. Within this zone, the reaction layer is decreasingly represented by Peters' flamelet formulation [5] with an increasing ψ_α . Since a lower Z_{st} will lead to a larger transition region, the claim that an over-predicted $(\Delta Z)_R$ will result in a more restrictive regime diagram is hereby substantiated.

Recognizing that the ordinate and diagonal $\Delta = \eta_K$ indicate the grid resolution relative to the reaction-zone thickness and smallest turbulent length, respectively, the diagram can be divided according to the level of numerical fidelity. These divisions are addressed by the terms *DNS* and *LES* in Fig. 3, which the initial indicates a grid resolution that either resolves both characteristic length-scales or at least the Kolmogorov length-scale when a combustion model is implemented.

Two properties of the regime diagram are distinguished. First, a mere change in grid resolution will result in only a horizontal shift on the figure, thus not altering the regime categorization. However, the

1
2
3 fidelity of the simulation will obviously be affected, moving closer to or further from a DNS. Second, keeping
4 the grid resolution constant, a shift away from Peters' regime can be attributed to: (i) a thicker flame (a
5 diagonal shift with constant Δ/η_K); or (ii) a higher turbulent Reynolds number (a vertical shift). Since the
6 two effects are not mutually exclusive, a regime transition is more likely due to a combination of both.
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Figure 3: Multi-dimensional flamelet regime diagram satisfying condition (15). The local grid resolution decreases from the left to the right quadrant. The numbers correspond to the distribution of the regime diagram into physical space, which is applied in Fig. 7. For convention, all odd labels refer to regions where the flamelet model is applicable. Note, however, that the abscissa is not a hard cut-off for the validity of flamelet model since the region within $2Z_{st} \leq \psi_\alpha \leq 1$ is a transition zone. The upper limit of $Ka_K = 100$ is according to Ref. [5].

One caveat to Fig. 3 is its implicit assumption that:

$$0.005 \leq Z_{st} \leq 0.5 . \quad (15)$$

This is a reasonable range of the stoichiometric mixture fraction for typical diffusion flames. Below the range of stoichiometric mixture fraction, the two diagonals crossing $Ka_K = 1$ and $Ka_K = 100$ will both fall under the center diagonal of Fig. 3, which crosses $\psi_\alpha = 1$. As a result, the aforementioned transition region will grow and overlap with a larger range of Karlovitz number. Conversely, the same two diagonals will lie above the center diagonal, eliminating the entire transition region such that Peters' flamelet formulation may not apply unless $Ka_K \ll 1$. In this case, the reaction zone may physically be too thick for the flamelet concept, which builds on a “thin reaction-zone assumption” [15], to remain valid.

2.3. Regime Diagram for LES Application

In relation to the objective of using the flamelet regime diagram in the context of LES, one should recognize that the discussion thus far considers only the DNS formulation. This scope of just DNS directly follows the equation sets (1) or (4), where all terms are unfiltered and the SGS terms are absent. The rotated transport equations for typical LES applications are:

$$\begin{aligned} \frac{\partial \widetilde{Y}_\alpha}{\partial t} + \widetilde{U}_j \frac{\partial \widetilde{Y}_\alpha}{\partial X_j} &= \frac{-1}{\bar{\rho}} \frac{\partial}{\partial X_j} \left[\bar{\rho} \widetilde{V}_{\alpha,j} \widetilde{Y}_\alpha \right] + \widetilde{\omega}_\alpha \\ &\quad - \frac{1}{\bar{\rho}} \frac{\partial}{\partial X_j} \left[\bar{\rho} \left((U_j Y_\alpha)'' + (V_{\alpha,j} Y_\alpha)'' \right) \right], \end{aligned} \quad (16a)$$

$$\begin{aligned} \frac{\partial \widetilde{Z}}{\partial t} + \widetilde{U}_1 \frac{\partial \widetilde{Z}}{\partial X_1} &= \frac{1}{\bar{\rho}} \frac{\partial}{\partial X_j} \left[\bar{\rho} \widetilde{D}_Z \frac{\partial \widetilde{Z}}{\partial X_j} \right] \\ &\quad - \frac{1}{\bar{\rho}} \frac{\partial}{\partial X_j} \left[\bar{\rho} \left((U_j Z)'' - \left(D_Z \frac{\partial Z}{\partial X_j} \right)'' \right) \right], \end{aligned} \quad (16b)$$

where the turbulent fluxes $(\alpha\beta)'' = \widetilde{\alpha\beta} - \widetilde{\alpha}\widetilde{\beta}$ and the local frame rotation is implemented with respect to the filtered mixture-fraction gradient instead:

$$\frac{\partial \widetilde{Z}}{\partial X_j} = \left[\left| \frac{\partial \widetilde{Z}}{\partial x_i} \right|, 0, 0 \right]^T, \quad (17a)$$

$$\frac{\partial}{\partial X_j} = \left(\frac{1}{|\nabla \widetilde{Z}|^2} \frac{\partial \widetilde{Z}}{\partial X_j} \right) \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial}{\partial x_i} + \nabla_j^\perp. \quad (17b)$$

Comparing Eqs. (16) to Eqs. (4) and (5), the individual terms, except the turbulent fluxes, are clearly in correspondence regardless of the Favre-filter operator, $(\cdot)$. In fact, Chan [25] and Wang [26] have independently derived a filtered version of the flamelet equation (8) where the turbulent fluxes only act as additional source terms. These observations indicate that the regime parameter, ψ_α , can be estimated by the resolved terms of LES:

$$\psi_\alpha \approx \frac{\sum_{j=2}^3 -\frac{\partial}{\partial X_j} \left[\bar{\rho} \widetilde{V}_{\alpha,j} \widetilde{Y}_\alpha \right] - \frac{\partial}{\partial X_j} \left[\bar{\rho} \widetilde{D}_Z \frac{\partial \widetilde{Z}}{\partial X_j} \right] \frac{\partial \widetilde{Y}_\alpha}{\partial \widetilde{Z}}}{-\frac{\partial}{\partial X_1} \left[\bar{\rho} \widetilde{V}_{\alpha,1} \widetilde{Y}_\alpha \right] - \frac{\partial}{\partial X_1} \left[\bar{\rho} \widetilde{D}_Z \frac{\partial \widetilde{Z}}{\partial X_1} \right] \frac{\partial \widetilde{Y}_\alpha}{\partial \widetilde{Z}}}, \quad (18)$$

where:

$$\frac{\partial}{\partial \widetilde{Z}} = \left(\frac{\partial \widetilde{Z}}{\partial X_1} \right)^{-1} \frac{\partial}{\partial X_1}. \quad (19)$$

The approximation of Eq. (18) can be explained mathematically by noting that the regime parameter is essentially a ratio of diffusion effects in the flame-aligned direction to that in the flame-orthogonal direction. Scalar diffusion, on the other hand, is intrinsically related to the second-order derivatives of the scalar profile, which in general decreases upon filtering. However, this reduction depends on the magnitude of each

component of the scalar gradient and therefore is not necessarily isotropic. To further substantiate this idea, an analysis with a two-dimensional test function was performed and presented in [Appendix B](#).

Another consideration with regard to typical LES is the ambiguity of the filter function in such simulations. Wang [26] suggested that a filtering treatment essentially extracts the principal features of an unfiltered field at the resolved scale. With this property, the filter function should preserve most of the (mis)alignment of the mixture fraction and species fields, thus increasing the accuracy of the approximation in Eq. (18). Therefore, even though the use of a homogeneous top-hat filter in the previous example and results in Sec. 4 do not exactly reflect the filtering in LES, such implementation should present a more critical assessment of the regime diagram than using *a posteriori* LES data.

3. DNS Configuration

The configuration of interest is a DNS of a turbulent lifted hydrogen jet flame in a heated coflow. This configuration was studied by Yoo *et al.* [18]. The DNS was performed at a jet Reynolds number of 8000, based on mean fuel injection velocity of 240 m/s, jet width of 2 mm, and fuel viscosity of 6×10^{-5} m²/s. The computational domain of the flame is a three-dimensional box with dimensions of $30 \times 40 \times 6$ mm³ in streamwise, transverse, and spanwise directions, respectively. The domain is discretized by a Cartesian grid of $2000 \times 1600 \times 400$ points in order to fully resolve all scales of the turbulent flow. The reaction chemistry was represented by a detailed hydrogen-air chemical kinetic mechanism, which consists of nine species and 21 elementary reactions [27]. The thermodynamic and mixture-averaged transport properties of the species were calculated with the CHEMKIN and TRANSPORT software libraries [28, 29], respectively.

The instantaneous temperature profile from the DNS for time $t = 1.5$ ms, along with its corresponding filtered profiles for $\Delta/\Delta_{\text{DNS}} = \{8, 32, 128\}$ are shown in Fig. 4(a). The stoichiometric hydroxyl mass-fraction and temperature along the streamwise direction for the four profiles are illustrated in the top and bottom subplots of Fig. 4(b), respectively. For reference, each filter is indicated in Fig. 4(a) by a blue bar and in Fig. 4(b) by a shaded area, in which the color-intensity is proportional to the width.

4. A-Priori Analysis Results

In the following, results from *a priori* analyses using the regime diagram developed in Sec. 2 will be presented. Both the unfiltered and filtered DNS data, as shown in Fig. 4, will be used to assess the implementation of the diagram in the DNS and LES regimes. The Kolmogorov length-scale is estimated with the calculated value of the regime parameter and estimation of the reaction-zone thickness:

$$\delta_R = \frac{(\Delta Z)_R}{|\nabla Z|}, \quad (20)$$

(a) Temperature field at the centerplane for four grid-resolutions. The contour line denotes the location of stoichiometric mixture fraction.

(b) Stoichiometric (top) hydroxyl mass-fraction and (bottom) temperature along the streamwise direction in the centerplane.

Figure 4: Variation of the centerline scalar profiles with respect to the filter size. Note that only half of the plane is shown due to the configuration's property of statistical symmetry in y -direction.

with further details given in Sec. 4.3. Through these evaluations, the generality of the regime parameter, along with its approximation using filtered information of the resolved scale will be demonstrated. In addition, the regime diagram will be employed for guidance of LES grid-refinement, indicating a practical use of the method other than being a diagnostic tool.

4.1. Dependence on Species

For this section, only the unfiltered DNS data (cf. top-left plot of Fig. 4(a)) is considered. The scatter plots in the flamelet regime space for the species H_2O , O_2 , OH , and HO_2 are shown, from top to bottom, in Fig. 5. Note that the figure corresponds to the unfiltered DNS data shown in Fig. 4(a) and is colored by temperature. Despite their correspondence to different species (both major and intermediate), all scatter plots exhibit qualitative similarities.

Figure 5: Scatter data in the flamelet regime diagram (left) and the PDF (right) for H_2O , O_2 , OH , and HO_2 profiles from top to bottom rows. The lower and upper dashed lines in the scatter plot denote $\text{Ka}_K \leq 1$ and $\text{Ka}_K > 100$, respectively. All plots are colored by temperature. The number in the PDF refers to the percentage of the scatter data that satisfies the range $\psi_\alpha \leq 1$.

The scatter plots are mostly confined to the left-half of the regime diagram, below the main diagonal that

indicates $\Delta/\eta_K = 1$. This uneven distribution of points is expected because the current dataset corresponds to the DNS, in which all relevant scales of the flow are well resolved. The small number of points that lie above the diagonal of $\Delta/\eta_K = 1$ is associated with regions of lower temperature, which mostly occur upstream in accordance with Fig. 4(b). Due to high intensity turbulence that is common to these locations, the DNS there is slightly under-resolved [18], possibly contributing to the scatter above the $\Delta/\eta_K = 1$ line.

In addition, the plots indicate a general decrease in Δ/δ_R (i.e. increase in relative grid-resolution) with increasing temperature. Referring to Fig. 4, the temperature in general increases along the streamwise direction. Since the shearing and straining of the jet mixing-layer decrease with increasing streamwise distance, flamelets will consequently extend, resulting in thicker reaction-zones and hence a reduction in Δ/δ_R . Besides the reaction-zone thickness, the higher temperature is also associated with larger turbulent eddies at the smallest scale (i.e. decrease in Δ/η_K). This indication of a growth in the smallest turbulent structures is physical because the higher temperature will typically lead to an increase in turbulence dissipation (i.e. higher flow viscosity). Overall, the analysis of the scatter data using the regime diagram accurately describes a relaxation in the grid-resolution that is necessary to resolve all relevant scales with higher temperature and at further downstream locations.

Another feature shared by the scatter plots of Fig. 5 is the large distribution of points with $\psi_\alpha \leq 1$. Therefore, a dominant portion of the flame is represented by the classical flamelet regime [5]. In order to extract quantitative insight from the regime diagram, probability-density functions (PDFs) of the scatter plots are included in the right column of Fig. 5. Regardless of the species, the PDFs indicate that: (i) the most probable ψ_α is between the order of 0.1 and 1; and (ii) approximately 80% of the scatter is within the range of $\psi_\alpha \leq 1$. Additionally, the depiction of the PDFs in terms of temperature further reveals that the points that correspond to temperature above 1900 K are the major contributors shaping the density functions. In contrast, the non-reacting, cold regions occupy only approximately 15% of the scatter and spread more about $10^{-2} \lesssim \psi_\alpha \lesssim 10^0$.

Therefore, based on the similarities among the representative group of species, as discerned in Fig. 5, the following evaluations can be performed with just H_2O data without a loss of generality. In addition, this generality essentially substantiates the length-scale argument that has been presented in Sec. 2.2.

4.2. Effects of Filter-Width

This section will investigate the implementation of the flamelet regime diagram in LES settings using *a priori* analyses with various filtered DNS datasets. Three filters, $\Delta/\Delta_{\text{DNS}}$, of $\{8, 32, 128\}$ are employed, and the corresponding filtered temperature contours and stoichiometric temperature along the streamwise direction are illustrated in Fig. 4. The flamelet regime scatter plots and PDFs for the original and three

filtered H_2O profiles are shown in Fig. 6. Note that the findings are applicable to other species, as has been demonstrated in Sec. 4.1.

Figure 6: Scatter in the flamelet regime diagram (left) and the scatter's PDF (right) for H_2O profile with $\Delta/\Delta_{\text{DNS}} = \{1, 8, 32, 128\}$, in order of top to bottom rows. Refer to Fig. 5 for more details.

The scatter plots shown in Fig. 6 suggest that moderate filter size of $\Delta/\Delta_{\text{DNS}} = 8$ has a mild effect on the spreading of $\psi_{\text{H}_2\text{O}}$. This finding is particularly clear by comparing the PDFs, which show, regardless of filtering, that: (i) the most probable $\psi_{\text{H}_2\text{O}}$ is between the order of 0.1 and unity; and (ii) more than 70% of the scatter is within the range of $\psi_{\text{H}_2\text{O}} \leq 1$. In other words, using the approximation of ψ_α by Eq. (18), the filtered DNS results of $\Delta/\Delta_{\text{DNS}} = 8$ will indicate that a dominant portion of the flame is represented by the classical flamelet regime [5]. This observation is consistent with the results from the original DNS data, as discussed in the preceding section. The agreement between the unfiltered case and filtered case of $\Delta/\Delta_{\text{DNS}} = 8$ is expected, since most of the flow features are still resolved by the coarser resolution, as seen from the corresponding temperature profiles in Fig. 4(a).

Considering the horizontal distribution of the scatter plots of Fig. 6, one can discern that the points for the filtered case with $\Delta/\Delta_{\text{DNS}} = 8$ spread across both halves of the regime diagram, in contrast to the

unfiltered results. Consequently, only regions of high temperature (~ 2000 K) are resolved by the coarser grid. However, the decrease in Δ/δ_R with increasing temperature remains clear in the filtered results. Therefore, the underlying physics can still be accurately captured by the flamelet regime diagram even with a filter of $\Delta/\Delta_{\text{DNS}} = 8$.

With regards to the cases of $\Delta/\Delta_{\text{DNS}} = \{32, 128\}$ of Fig. 6, further loss of information tends to cumulate the scatter of $\psi_{\text{H}_2\text{O}}$ about the unity-order magnitude, leading to an overall shift of the PDFs towards higher values of $\psi_{\text{H}_2\text{O}}$. This shift can be quantified by the decrease in the percentage of scatter within the range of $\psi_{\text{H}_2\text{O}} \leq 1$ to approximately 66%. This congregation of points can be attributed to the equalization of diffusion in the mixture-fraction gradient and its orthogonal directions due to increasing filter effects, a phenomenon that is also observed for the test case shown in Fig. B.8. Hence, the accuracy of the approximation by Eq. (18) will deteriorate with increasing filter-width, so caution should be taken for the implementation of the one-dimensional flamelet regime with excessively coarsened grids. However, the majority of scatters (over 60%) being within the range of $\psi_{\text{H}_2\text{O}} \leq 1$ suggests that the analysis may still serve as a robust estimate for the flamelet regime of a reacting flow using significantly under-resolved results. In other words, with grid coarsening, the turbulence-chemistry interactions of the current configuration can be approximated by the flamelet model, but the details on flame structures and multi-dimensional effects will be lost.

In comparison to the case with $\Delta/\Delta_{\text{DNS}} = 8$, the scatter data of the cases with $\Delta/\Delta_{\text{DNS}} = \{32, 128\}$ occupy only the right-half of the regime diagram, indicating that the two lower grid-resolutions are insufficient to resolve the reaction-zone thickness anywhere within the domain. A small, but high-temperature part of the $\Delta/\Delta_{\text{DNS}} = 32$ scatter, however, remains smaller than the Kolmogorov length-scale, while all points of $\Delta/\Delta_{\text{DNS}} = 128$ are larger than the smallest turbulent scale. Interestingly, both cases with larger filter-width retain the association of low Δ/δ_R with high temperature, and vice versa, as discussed in the cases with $\Delta/\Delta_{\text{DNS}} = \{1, 8\}$ of Fig. 6.

From the various cases of Fig. 6, a notable trend is the reduction in the range of temperature as the filter-width increases. This reduction is justified and attributed to the smoothing and redistributing properties of a spatial-filter, which can be clearly seen from the stoichiometric temperature profiles for the various cases shown in Fig. 4(b).

4.3. Estimation of Kolmogorov Length-Scale

The scaling analysis presented in Sec. 2.2 suggests that the Kolmogorov length-scale of the planar lifted jet flame can be estimated with a given reaction-zone thickness. Table 1 lists the minimum/maximum Kolmogorov lengths corresponding to the cases that have been evaluated in Secs. 4.1 and 4.2. Per Eq. (20),

the reaction-zone thickness of a flamelet in Tab. 1 is calculated by dividing $(\Delta Z)_R \approx 2Z_{\text{st}}$ by the maximum L^2 -norm of the mixture-fraction gradient. The latter is related to the scalar dissipation rate by inverting Eq. (9): $|\nabla Z| = \sqrt{\chi_Z/2D_Z}$. Due to this representation by the maximum mixture-fraction gradient norm, the range of reaction-zone thickness in Tab. 1 is common to all species. For the filtered cases, the gradient norm is calculated from the *total* scalar dissipation rate:

$$|\nabla Z| \approx \sqrt{\widetilde{\chi_Z/2D_Z}} = \left| \nabla \widetilde{Z} \right| + \sqrt{\chi_{Z,\text{SGS}}/2D_Z}. \quad (21)$$

Note that, in LES, the SGS contribution on the right-hand-side will be given by the turbulence model.

	Reaction-Zone Thickness δ_R [μm]	Kolmogorov Length η_K [μm]
$\Delta/\Delta_{\text{DNS}} = 1$		
H ₂ O	28 - 2750	0.34 - 381
O ₂		0.24 - 540
OH		0.98 - 543
HO ₂		1.7 - 2080
H ₂ O		
$\Delta/\Delta_{\text{DNS}} = 8$	33 - 2120	0.91 - 436
$\Delta/\Delta_{\text{DNS}} = 32$	52 - 1670	1.6 - 167
$\Delta/\Delta_{\text{DNS}} = 128$	88 - 552	6.8 - 95

Table 1: Quantification of the reaction-zone thickness and Kolmogorov length for the cases evaluated in Figs. 5 and 6.

For a reaction-zone thickness given by the unfiltered dataset, the Kolmogorov length evaluated from the flamelet regime parameter is seen to vary within the range of $\mathcal{O}(10^{-2}\Delta_{\text{DNS}})$ to $\mathcal{O}(10^2\Delta_{\text{DNS}})$ regardless of the species, where $\Delta_{\text{DNS}} \approx 20 \mu\text{m}$. The four orders-of-magnitude range of η_K is acceptable because of the considerable spatial variations of the turbulence Reynolds number of the current configuration, which comprises both laminar and turbulent flows. Furthermore, noting that: (i) the minimum Kolmogorov length estimated by Yoo *et al.* [18] is of $\mathcal{O}(0.5\Delta_{\text{DNS}})$, which agrees reasonably with the lowest estimation in the current study; and (ii) the various estimations by different species are consistently within a factor of order unity among each other; the length-scale argument for the scaling of ψ_α (cf. Sec. 2.2) is therefore supported.

Referring to the filtered cases of $\Delta/\Delta_{\text{DNS}} = \{8, 32, 128\}$ for H₂O, the ranges of both the reaction-zone thickness and Kolmogorov length narrow as the filter-width increases because of the stronger smoothing and redistributing effects of wider spatial-filters. Based on the generally monotonic increase of the minimum δ_R and decrease of the maximum η_K , one can infer that the range of the flamelet regime parameter range will remain relatively constant. Hence, the applicability of the approximation of ψ_α via Eq. (18), first assessed in Sec. 4.2, is again demonstrated, particularly for such moderate filter-widths as $\Delta/\Delta_{\text{DNS}} = 8$.

The flamelet regime analysis also serves as a reasonable indicator of the order of the Kolmogorov length considering the proximity between the η_K range of the evaluated cases.

4.4. Guidance for LES Model Selection

The ability of the flamelet regime analysis to provide information about the grid-resolution relative to the reaction-zone thickness and Kolmogorov length (cf. Secs. 4.2 and 4.3) suggests that the regime diagram may be used as a guiding tool for model selection in LES. In order to do so, the flamelet regime diagram shown in Fig. 3 are divided into four segments. The regimes labeled as “1” and “2” denote the DNS regime and “3” and “4” refer to the LES regime. The odd and even labels represent the range $\psi_\alpha \leq 1$ and $\psi_\alpha > 1$, respectively. In addition, the non-reacting portions of the flow will be labelled as “0”. The distribution of the four flamelet regimes in physical space is shown in Fig. 7 for the original DNS data, along with its three filtered cases of $\Delta/\Delta_{\text{DNS}} = \{8, 32, 128\}$. Note that the results in Fig. 7 are evaluated from $\psi_{\text{H}_2\text{O}}$ and the shaded columns at the left and right extremes are regions that are not considered in this analysis.

Figure 7: Distribution of the flamelet regime diagram segment labels along the centerline plane for four grid-resolutions. The contour line denotes the location of stoichiometric mixture fraction. The shaded columns at the left and right extremes were excluded in this analysis.

For the unfiltered DNS dataset, the planar jet flame is dominantly occupied by segment 0 and 1, thus

confirming the discussion in Sec. 4.1 that this flame configuration can be represented by the flamelet regime. Localized regions of segment 2, in which the flamelet formulation is inapplicable, can be discerned throughout the domain, occurring generally in the fuel-rich part of the jet. More importantly, the dominance of segments 1 and 2 confirm that the flame is well-resolved by the unfiltered DNS grid-resolution (which is expected for a DNS), so no combustion model will be needed in this case.

Similarly, the moderately filtered case of $\Delta/\Delta_{\text{DNS}} = 8$ appears to be mostly occupied by segment 0 and 1, along with scattered regions of segment 2. Additionally, there are some unresolved regions denoted by segment 3 and 4, which are mainly confined to the upstream part of the flame (up to five jet-width distance). The congregation of insufficiently resolved regions at the upstream vicinity indicates a stronger requirement on grid-density if no closure model were to be provided there to represent the turbulent-combustion phenomena. This condition is consistent with the placement of grid points by conventional meshing practice in DNS. Also, the multi-dimensional flamelet segments 2 and 4 are typically located at the fuel-rich part of the flame, where the latter will invalidate the use of the classical flamelet model [15] and demand a combustion model that can account for the multi-dimensional flamelet effects.

For the cases with $\Delta/\Delta_{\text{DNS}} = \{32, 128\}$, most of the domain is occupied by the unresolved segments 3 and 4, indicating that the grid-resolution is too low to fully resolve any relevant length-scales of the planar jet flame. Therefore, the implementation of turbulence and combustion models become extremely important so that the under-resolving LES can still generate representative filtered results.

In summary, given a level of grid resolution, we can use the flamelet regime diagram to analyze if a combustion model is necessary and, if so, whether the classical flamelet model [15] is suitable. For the initial consideration, a lack of a need in combustion models may indicate that the grid-resolution is excessive for a LES. For the latter assessment, any localized inapplicability of the classical flamelet model has to be compensated by either: (i) using another combustion model that can describe the multi-dimensional flamelet effects; or (ii) adaptive mesh refinement so that a combustion model becomes unnecessary. A caveat to these two remedies is the potential need for an interface that allows for the coupling among different combustion models, constituting a hybrid-type combustion model [30].

5. Conclusions

This study developed a flamelet regime diagram that evaluates the applicability of various diffusion flamelet models with respect to the grid-resolution and flow conditions. Noteworthy of the regime diagram is the definition of its two parameters, both of which can be evaluated in turbulent diffusion flames.

Using length-scale arguments based on the concepts of inner-reaction zone thickness and dissipation

element, the regime diagram relates to the Karlovitz number defined for non-premixed flames and identifies regions where the conventional one-dimensional flamelet model is applicable. The flamelet regime diagram was assessed through *a priori* analyses of a direct numerical simulation dataset that corresponds to a planar turbulent lifted hydrogen jet flame in a heated coflow.

The length-scale arguments were substantiated by the finding that the regime parameter is of similar order-of-magnitude among different species. By filtering the direct numerical simulation data, the finding that the prevalence of one-dimensional flamelets is generally unchanged with filter-width is observed. This observation agrees with the consistency requirement on a regime diagram, which states that the fundamental combustion mode is not dependent on the filter-width. This result also verified that the approximation of the regime parameter using information from only the resolved scales of large-eddy simulations is reasonable. Additionally, the analysis with the explicitly filtered data highlighted the potential use of the flamelet regime diagram as a practical guide for turbulent-combustion model selection.

Further work for this study is the *a posteriori* assessment of the flamelet regime diagram, which is a consideration for future research. Specifically, the possibility of an invalidation of the flamelet formulation by the regime diagram based on large-eddy simulation results generated with a flamelet-model closure will be a noteworthy question to answer.

Appendix A. Equation Derivations

In this section, relevant equations of the main document will be discussed in details to aid the understanding of the development and validity of the mathematical formulations.

Beginning with the rotated species transport equation (4), the left-hand-side (LHS) of this equation can be substituted by Eq. (6b), thus giving:

$$\begin{aligned} \frac{\partial Y_\alpha}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial Y_\alpha}{\partial Z} + U_1 \frac{\partial Y_\alpha}{\partial X_1} &= \frac{\partial Y_\alpha}{\partial \tau} + \left(\frac{\partial Z}{\partial t} + U_1 \frac{\partial Z}{\partial X_1} \right) \frac{\partial Y_\alpha}{\partial Z} \\ &= \frac{\partial Y_\alpha}{\partial \tau} + \frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\rho D_Z \frac{\partial Z}{\partial X_j} \right] \frac{\partial Y_\alpha}{\partial Z}. \end{aligned} \quad (\text{A.1})$$

Moving the second term on the right-hand-side (RHS) of Eq. (A.1) to the LHS of Eq. (4), we obtain:

$$\begin{aligned} \frac{\partial Y_\alpha}{\partial \tau} &= D_Z \frac{\partial Z}{\partial X_j} \frac{\partial}{\partial X_j} \left[\frac{1}{\text{Le}_\alpha} \frac{\partial Y_\alpha}{\partial Z} \right] + \frac{1}{\rho} \left(\frac{1}{\text{Le}_\alpha} - 1 \right) \frac{\partial}{\partial X_j} \left[\rho D_Z \frac{\partial Z}{\partial X_j} \right] \frac{\partial Y_\alpha}{\partial Z} + \omega_\alpha \\ &\quad + \frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\frac{\rho D_Z}{\text{Le}_\alpha} \nabla_j^\perp Y_\alpha \right] + \frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\rho \left(-V_{\alpha,j} Y_\alpha - D_\alpha \frac{\partial Y_\alpha}{\partial X_j} \right) \right]. \end{aligned} \quad (\text{A.2})$$

Applying the transformation (3c) on the first and second terms on the RHS of Eq. (A.2), and replacing terms with the definitions of scalar dissipation rate and curvature of the mixture-fraction field stated in

Eqs. (9) and (10), we will then arrive at the multi-dimensional species flamelet equation (8) of Sec. 2.1. Note that the mixture-fraction curvature equation (10) is derived as:

$$\begin{aligned}
\kappa_Z &= -\frac{\partial}{\partial x_i} [\hat{n}_i] = -\frac{\partial}{\partial X_j} \left[\frac{1}{|\nabla Z|} \frac{\partial Z}{\partial X_j} \right] \\
&= \frac{1}{|\nabla Z|^2} \frac{\partial |\nabla Z|}{\partial X_1} \frac{\partial Z}{\partial X_1} - \frac{1}{|\nabla Z|} \frac{\partial}{\partial X_j} \left[\frac{\partial Z}{\partial X_j} \right] \\
&= \frac{1}{|\nabla Z|} \left(\frac{\partial |\nabla Z|}{\partial X_1} - \sum_{j=1}^3 \frac{\partial^2 Z}{\partial X_j^2} \right) \\
&= \frac{-1}{|\nabla Z|} \sum_{j=2}^3 \frac{\partial^2 Z}{\partial X_j^2} = \frac{-1}{|\nabla Z|} \frac{\partial}{\partial X_j} [\nabla_j^\perp Z] .
\end{aligned} \tag{A.3}$$

In order to bring Eq. (8) to the form presented in Ref. [14], the final term of Eqs. (8) and (A.2) can be expanded as:

$$\begin{aligned}
&\frac{\partial}{\partial X_j} \left[\rho \left(-V_{\alpha,j} Y_\alpha - D_\alpha \frac{\partial Y_\alpha}{\partial X_j} \right) \right] \\
&= \frac{\partial}{\partial X_j} \left[\frac{\rho D_Z Y_\alpha}{\text{Le}_\alpha W} \frac{\partial W}{\partial X_j} - \sum_\beta \frac{\rho D_Z Y_\alpha}{\text{Le}_\beta} \left(\frac{\partial Y_\beta}{\partial X_j} + \frac{Y_\beta}{W} \frac{\partial W}{\partial X_j} \right) \right] \\
&= \underbrace{\frac{\rho \chi_Z Y_\alpha}{2 \text{Le}_\alpha W} \frac{\partial^2 W}{\partial Z^2}}_{\mathcal{J}_{\alpha,1}^{WZ}} \\
&\quad + \underbrace{\left[\frac{\rho \chi_Z Y_\alpha}{2 W} \frac{\partial}{\partial Z} \left[\frac{1}{\text{Le}_\alpha} \right] + \frac{1}{4 \text{Le}_\alpha} \left(\frac{\partial}{\partial Z} \left[\rho \chi_Z \frac{Y_\alpha}{W} \right] + \frac{\chi_Z}{D_Z} \frac{\partial}{\partial Z} \left[\rho D_Z \frac{Y_\alpha}{W} \right] \right) \right]}_{\mathcal{J}_{\alpha,2}^{WZ}} \frac{\partial W}{\partial Z} \\
&\quad - \sum_\beta \frac{\rho \chi_Z Y_\alpha}{2 \text{Le}_\beta} \left[\frac{\partial^2 Y_\beta}{\partial Z^2} + \frac{Y_\beta}{W} \frac{\partial^2 W}{\partial Z^2} \right] \\
&\quad - \sum_\beta \left[\frac{\rho \chi_Z Y_\alpha}{2} \frac{\partial}{\partial Z} \left[\frac{1}{\text{Le}_\beta} \right] + \frac{1}{4 \text{Le}_\beta} \left(\frac{\partial \rho \chi_Z Y_\alpha}{\partial Z} + \frac{\chi_Z}{D_Z} \frac{\partial \rho D_Z Y_\alpha}{\partial Z} \right) \right] \frac{\partial Y_\beta}{\partial Z} \\
&\quad - \sum_\beta \left[\frac{\rho \chi_Z Y_\alpha Y_\beta}{2 W} \frac{\partial}{\partial Z} \left[\frac{1}{\text{Le}_\beta} \right] \right. \\
&\quad \quad \left. + \frac{1}{4 \text{Le}_\beta} \left(\frac{\partial}{\partial Z} \left[\rho \chi_Z Y_\alpha \frac{Y_\beta}{W} \right] + \frac{\chi_Z}{D_Z} \frac{\partial}{\partial Z} \left[\rho D_Z Y_\alpha \frac{Y_\beta}{W} \right] \right) \right] \frac{\partial W}{\partial Z} \\
&\quad + \underbrace{\frac{\partial}{\partial X_j} \left[\frac{\rho D_Z Y_\alpha}{\text{Le}_\alpha W} \nabla_j^\perp W \right]}_{\mathcal{J}_\alpha^{W\perp}} - \underbrace{\frac{\rho}{\text{Le}_\alpha} \sqrt{\frac{\chi_Z D_Z}{2}} \kappa_Z \frac{Y_\alpha}{W} \frac{\partial W}{\partial Z}}_{\mathcal{J}_\alpha^{W\kappa}} \\
&\quad - \sum_\beta Y_\alpha \frac{\partial}{\partial X_j} \left[\frac{\rho D_Z}{\text{Le}_\beta} \left(\nabla_j^\perp Y_\beta + \frac{Y_\beta}{W} \nabla_j^\perp W \right) \right] \\
&\quad + \sum_\beta Y_\alpha \left[\frac{\rho}{\text{Le}_\beta} \sqrt{\frac{\chi_Z D_Z}{2}} \kappa_Z \left(\frac{\partial Y_\beta}{\partial Z} + \frac{Y_\beta}{W} \frac{\partial W}{\partial Z} \right) \right]
\end{aligned} \tag{A.4a}$$

$$-\sum_{\beta} \nabla_j^{\perp} Y_{\alpha} \left[\frac{\rho D_Z}{\text{Le}_{\beta}} \left(\nabla_j^{\perp} Y_{\beta} + \frac{Y_{\beta}}{W} \nabla_j^{\perp} W \right) \right], \quad (\text{A.4b})$$

where the summation terms are correction terms for mass conservation, with $\mathcal{J}_{\alpha}^{CZ}$ and $\mathcal{J}_{\alpha}^{C\perp}$ denoting, respectively, the terms with *only* derivative in Z and those related to κ_Z and $\nabla_j^{\perp}$.

Appendix B. LES Regime Parameter Approximation

In Sec. 2.3, the regime parameter in the context of LES is suggested to be reasonably estimated by only the resolved terms. Here, we demonstrate this concept with a two-dimensional test function, $f = f(x, y)$, plotted over a 256×256 square grid. This function is shown by the contour areas in Fig. B.8, where the function's gradient has generally larger x -component than the orthogonal y -component. The filtered test function, $\bar{f}$, is constructed with a homogeneous top-hat filter and illustrated, for the filter width of 64 grid spacings, in Fig. B.8 by the contour lines. The filtered function indicates that the general dominance of x -component over y -component is retained despite a reduction in its peak value due to filtering.

The changes in: (i) the function's peak value ($\max[f]$) and (ii) the ratio of second function derivative in y to that in x ($\partial_y^2 f / \partial_x^2 f$) with respect to the filter-width ($\bar{\Delta}$), normalized by the grid-spacing (Δ), are shown in the top- and bottom-right plots of Fig. B.8, respectively. The second derivative plot in Fig. B.8 shows three lines to denote the different ways in which the ratio can be evaluated. Regardless of the evaluation method, the second derivative ratio, $\partial_y^2 f / \partial_x^2 f$, exhibits only mild sensitivity to the increase in filter-width, remaining approximately of the same order-of-magnitude as given by the unfiltered function:

$$\frac{\partial^2 \bar{f}}{\partial y^2} \bigg/ \frac{\partial^2 \bar{f}}{\partial x^2} \sim \frac{\partial^2 f}{\partial y^2} \bigg/ \frac{\partial^2 f}{\partial x^2}. \quad (\text{B.1})$$

For the same reason, we can approximate ψ_{α} in case of LES using only the diffusion of resolved terms, as suggested in Eq. (18).

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Figure B.8: Two-dimensional test function (contour areas) and its filtered counterpart with filter width of 64 out of 256 grid spacings (contour lines), both colored by the profiles' values. The top- and bottom-right plots correspond to the change of the peak function value and ratio of second derivative in y to that in x with respect to grid-spacing, respectively. The three lines in the second-derivative ratio plot denote different evaluation methods: (i) $\max \left[\frac{\partial^2 f}{\partial y^2} \right] / \max \left[\frac{\partial^2 f}{\partial x^2} \right]$, $\square$; (ii) $\max \left[\frac{\partial^2 f}{\partial y^2} \right] / \max \left[\frac{\partial^2 f}{\partial x^2} \right]$, $\triangle$; and (iii) $\left\langle \frac{\partial^2 f}{\partial y^2} / \frac{\partial^2 f}{\partial x^2} \right\rangle$, $\circ$, where $\langle \cdot \rangle$ indicates an averaging procedure.

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