

LARGE-EDDY SIMULATION OF PARTIALLY PREMIXED TURBULENT COMBUSTION

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ABSTRACT

The development of successful modeling techniques for numerical simulations of technical combustion devices will help in the design of more efficient and more stable conversion of chemical into mechanical energy with lower emissions of harmful pollutants. Because of the intricate and complex coupling of chemistry with small-scale and large-scale fluid flow and mixing processes, combustion is inherently a multi-scale problem. For most of the important combustion regimes, the coupling of molecular mixing and chemistry leads to small-scale features, whose structures depend on the flow regime. These local flame structures need to be modeled adequately and incorporated into a large-scale model. Because of the strong non-linearities of the chemical production rates that can lead to the importance of rare events and because of the importance of scalar mixing for combustion, it will be shown that large-eddy simulations lead to strongly improved predictions for combustion processes. Here, the focus will be on partially premixed combustion, which is characterized by local flame structures in both the premixed and the non-premixed regime. We highlight and discuss some of the modeling challenges that are important for realistic combustion devices.

INTRODUCTION

Numerical simulations of technical combustion devices, such as aircraft or automotive engines are quite complex as they require an adequate description of liquid fuel injection and atomization, drop dynamics and evaporation, large-scale turbulent mixing and small-scale molecular mixing of fuel and air, chemical reactions, and turbulence/chemistry interactions. Many of these processes happen on multiple time and length scales, which creates a modeling challenge. Turbulent combustion is a prime example of a multi-scale problem. Obviously, turbulence at high enough Reynolds numbers already has a wide range of scales. But the range of chemical time-scales that is involved, for example, in the formation of pollutants is even wider. The interaction of chemistry with turbulent and molecular mixing not only involves all of these scales, but creates additional scales that are related to the production and consumption layers of chemical species and sensible energy. These flame scales directly involve molecular mixing, since in non-premixed flames, combustion only takes place if fuel and air are mixed on a molecular level, or, in premixed flames, when fresh unburned gases are heated up sufficiently by heat conduction from the burned gases. Therefore, in turbulent combustion, where molecular transport occurs almost exclusively on the smallest turbulent scales, the combustion process happens on the small scales too.

In combustion physics, one has to distinguish between

the premixed and the non-premixed combustion regimes. The different small-scale combustion physics in the premixed and non-premixed regimes need to be considered in a combustion modeling approach. Combustion models are therefore typically targeted to one of these regimes. For non-premixed turbulent combustion, several models have been proposed. It has long been recognized that in this regime, changes in chemistry tend to occur mostly with changes in the local equivalence ratio, and will often occur on a time-scale that is fast relative to the local flow time-scale. The local equivalence ratio can be expressed by the mixture fraction, which is defined to be zero in the pure oxidizer and unity in the pure fuel. From this result the mixture fraction based models, such as flamelet models [1] or the conditional moment closure models [2, 3, 4]. These models have in common that a local fluctuation of a reactive scalar is essentially decomposed into mostly a fluctuation in mixture fraction, which is a non-reactive scalar and therefore easy to model, plus a smaller contribution from the fluctuation of the reactive scalar with respect to the mixture fraction. In the flamelet model, this second part is modeled by solving the so called flamelet equations, which are derived from the governing equations by performing a coordinate transformation that replaces a spatial coordinate by the mixture fraction and a subsequent asymptotic analysis that assumes fast, but not infinitely fast chemistry. The flamelet equations describe the local flame structure, which results from the small-scale balance of chemistry and molecular transport, as function of the mixture fraction. These flame structures are incorporated into a model for the large-scale flow by using a presumed probability density function (pdf) for the mixture fraction that depends on its local mean and variance. This method computes the large-scale quantities, such as mean density, mean temperature, or mean species mass fractions by considering the small-scale structure of the flame. The flamelet model for non-premixed turbulent combustion therefore truly is a multi-scale approach.

Non-Premixed Combustion

Different implementations of the flamelet approach have been proposed in the past. Very interesting, because of their simplicity, are steady flamelet models. Here, the unsteady term in the flamelet equations is neglected. These equations then essentially have only one free parameter, which is the dissipation rate of the mixture fraction. The solutions of the flamelet equations can therefore be pre-computed and can be tabulated for later use in CFD simulations. In the conventional steady laminar flamelet model, all scalar quantities can be obtained from the flamelet table as function of the mean mixture fraction, the mixture fraction variance, and the mixture fraction dissipation rate. Here, we will focus on

a different variant of the steady flamelet model, the so called flamelet/progress variable (FPV) model proposed by Pierce and Moin [5]. In this model, an additional equation for a reaction progress variable is solved, and the mixture fraction dissipation rate is replaced by the progress variable as a parameter in the flamelet table. This is a feature that will be important in the development of a regime-independent model, since it is consistent with the models for premixed turbulent combustion discussed below. The fact that the pdf of the reaction progress variable is modeled as a delta function makes FPV a model that is particularly targeted towards LES, since this assumption is much less justifiable for Reynolds averaged quantities. Extensions of the model by Ihme and Pitsch [6, 7, 8], where both beta-function and the statistically most likely distribution have been used to describe the pdf of a reaction progress parameter might make the model also applicable in the Reynolds averaged context.

As long as the chemistry is not too slow, the models for turbulent non-premixed combustion are fairly robust, and there are two reasons for this. First, the reaction zone is typically very close to stoichiometric conditions, which corresponds to an iso-surface of mixture fraction, since for sufficiently fast chemistry, there is no fuel on one side and no oxygen on the other side of that surface. This implies that the flame location can be determined by the solution of a non-reactive scalar equation, which can be expected to be fairly accurate. Second, in the limit of fast enough chemistry, the heat release is mostly governed by the rate of molecular mixing of fuel and air, which is described by the dissipation rate of the mixture fraction. While it is not easy to accurately model dissipation rates, here again, the fact that only the dissipation rate of a non-reactive scalar is needed makes modeling much easier than if it was for a reactive scalar.

Premixed Combustion

For premixed turbulent combustion, there is no analogy to these simplifying features of non-premixed turbulent combustion. As a result, modeling premixed combustion is more challenging and typically less accurate. In premixed combustion, a reaction progress variable is often used to parameterize the combustion process and to localize the flame. A reaction progress variable can be defined from the reaction products or the temperature, and is often normalized to be zero in the unburned and unity in the burned region of the flow field. Then, a transport equation for the progress variable has to be solved, and closure for the reaction source term has to be provided. Most often, flamelet assumptions are used to close this term. An alternative to solving a progress variable equation is to use a level set equation to locate the flame position. The level set function is simply a scalar field that is defined such that an iso-surface of a given value is at the position of the flame. To give a concrete example, the level set function can be defined such that an iso-surface where the level set function is zero corresponds to the iso-surface of the temperature at the value of temperature of the reaction zone, which is called the inner layer temperature. The level set therefore describes the position of the flame. The definition of the level set away from the flame is within some constraints arbitrary, and therefore, no other physical meaning can be assigned to it. The equation describing the evolution of the level set is a kinematic equation, where the propagation of the flame comes from specifying a turbulent burning velocity, which is a quantity that needs to be modeled.

These and other models for non-premixed and premixed turbulent combustion have been validated or discussed in many studies. However, most technical combustion devices, although typically classified as premixed or non-premixed, have elements of both of these combustion regimes. It is therefore desirable to be able to use models that describe both combustion regimes and mixed partially premixed combustion modes. It is also important that such models still consider the local small-scale structure of the individual regimes correctly.

Large-Eddy Simulations for Turbulent Combustion

In large-eddy simulations (LES), the large, energy containing turbulent motions are resolved and directly computed, and the small-scale turbulent motions and their effects on the large scales have to be modelled. Because the combustion process occurs on the small scales of the turbulent motions, there is essentially no resolved part of the combustion process. Although the combustion process has to be modeled entirely, in the past, we have shown in many examples that large-eddy simulations provide much more accurate solutions for turbulent combustion problems than Reynolds-averaged Navier Stokes (RANS) modeling approaches [9, 10, 11]. The reason is that, because of the turbulence cascade, the small-scale turbulent motions and the small-scale molecular mixing process are very much governed by the large scales of the turbulence, which, using LES, is typically captured with good accuracy. Pitsch [10] showed for the example of a piloted jet flame that the consideration of fluctuations in the small-scale mixing rate predicted by LES, strongly improved the predictions of stable intermediates, such as carbon monoxide. Apparently, rare events of very high scalar dissipation rate are suppressed in rich partially premixed regions of the flame. Raman and Pitsch [11] performed large-eddy simulations of a bluff-body stabilized flame and demonstrated very good predictions of species mass fractions and temperature, which had not been achieved with any RANS-based approach. The analysis showed that the thin shear layers downstream of the bluff-body edge undergo Kelvin-Helmholtz instabilities and break down approximately one bluff-body diameter downstream of the nozzle. However, very rarely, this break-down occurs right at the edge of the bluff body and a large amount of air is entrained into the otherwise rich interior of the recirculation region just downstream of the bluff-body. These infrequent events change the dynamics of the flame, and it is obvious that such events cannot be predicted by Reynolds-averaged methods. Both these examples have in common that a highly non-linear process, in this case the turbulent combustion process involving the turbulence, the chemistry, and their interactions, is affected by rare infrequent events; and for strongly non-linear processes, even very rare events can change the first-order dynamics of the problem.

Several other phenomena of practical relevance that share these characteristics can be found in combustion devices. An example is the formation of soot in aircraft engines. Soot is formed in rich regions where the equivalence ratio is larger than about two. These rich regions typically exist in the primary combustion region, where as a consequence, large amounts of soot are usually formed. These regions form a sharp interface with the leaner regions, because of fast oxidation reactions mainly with OH. Further downstream, because of the introduction of secondary air, the equivalence ratio decreases, and most of the soot burns off. However, on rare occasions, a rich pocket survives the

secondary mixing region, which brings a large amount of soot into the exhaust. It could be speculated that a large fraction of particulate emissions from aircraft engines come from very few rich pockets with high soot volume fraction rather than from the bulk of the fluid.

In the present paper, we will discuss some of the challenges in turbulent combustion modeling. We will start by discussing dynamic sub-filter models for the scalar variance, which are particularly important in non-premixed combustion models. We will then discuss the particular challenges that arise in LES of premixed turbulent combustion when using reaction progress variable or level set methods. In this context, a level set formulation is developed that is coupled with a reaction progress variable equation. The model combines the strengths of both approaches and leads to improved numerical accuracy and a better description of the turbulent flame structure.

SCALAR VARIANCE MODELING IN NON-PREMIXED TURBULENT COMBUSTION

Non-premixed flamelet combustion models typically use scalar variance information to describe reactive source term and density fields. It is well known that the use of variance information is critical to the accurate prediction of combustion, but presently available variance models are prone to significant error. In an effort to reduce these errors, the fundamental assumptions that are used in formulating dynamic variance models are re-examined. This leads to a new method of calculating dynamic variance model coefficients [12]. It will be shown here in a priori tests using direct numerical simulations of scalar mixing that this new procedure leads to improved sub-grid variance predictions in constant density homogeneous turbulence.

New Formulation of the Dynamic Variance Calculation

An algebraic model for the mixture fraction variance can be formulated as

$$\overline{Z''^2} = C_4 \overline{\Delta}^2 |\nabla \overline{Z}|^2, \quad (1)$$

where C_4 is a model coefficient and $\overline{\Delta}$ is an LES filter width. A dynamic version of this model can be found by applying the well known Germano identity to Eq. (1) [13]. The resulting equation for the coefficient C_4 is

$$\overline{\overline{Z Z}} - \overline{\overline{Z}} \overline{\overline{Z}} = C_4 \left(\overline{\overline{\Delta}^2 \frac{\partial \overline{Z}}{\partial x_j} \frac{\partial \overline{Z}}{\partial x_j}} - \overline{\Delta}^2 \frac{\partial \overline{Z}}{\partial x_j} \frac{\partial \overline{Z}}{\partial x_j} \right), \quad (2)$$

where the right arrow represents a test filter. To test whether this coefficient could be accurately predicted by a dynamic procedure, a DNS of scalar mixing in homogeneous isotropic turbulence was performed by Balarac et al. [12]. The PDF of the C_4 coefficient from this DNS is shown parameterized by filter width in Fig. 1. It can be seen there that the PDF is bimodal, and peaks at both positive and negative values. This bimodal behavior is very difficult for dynamic procedures to describe, because these procedures can pick out only one coefficient value. One value can of course not accurately represent the physics that cause bimodal behavior. This implies that typical dynamic variance coefficient formulations are not very robust.

To determine the cause of this bimodality, the derivation of the dynamic procedure can be examined. Interestingly, Eq. (2) is found to be inconsistent with a Taylor-series

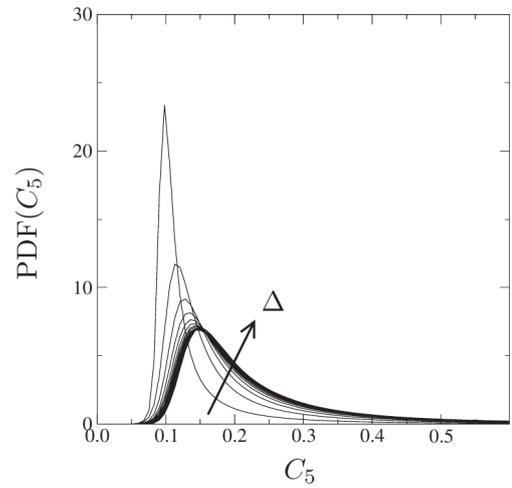
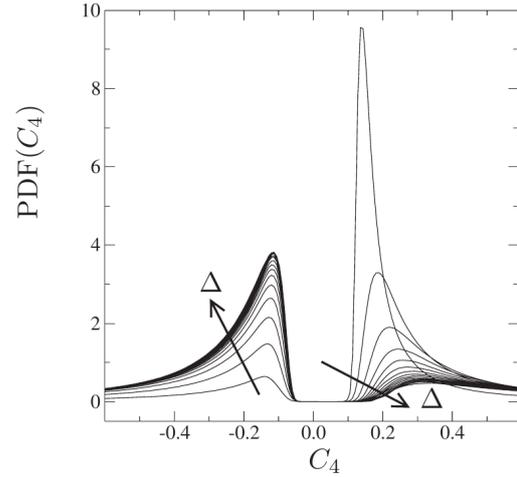


Figure 1: Plot of C_4 and C_5 for several filter sizes. The arrow indicates increasing filter size.

derived formulation of the model. A Taylor-series based approach instead led to a dynamic equation of the form,

$$\overline{\overline{Z Z}} - \overline{\overline{Z}} \overline{\overline{Z}} = C_5 \overline{\overline{\Delta}^2 \frac{\partial \overline{Z}}{\partial x_j} \frac{\partial \overline{Z}}{\partial x_j}}, \quad (3)$$

where C_5 is the associated model coefficient. The PDF of C_5 at several filter sizes is shown on the right hand side of Fig. 1. Unlike the C_4 PDF, the PDF of C_5 is unimodal with a distinct peak. The physics of this distribution are more easily captured by a dynamic procedure because a single coefficient is often a fair representation of a unimodal peak. This attribute makes the dynamic procedure shown in Eq. (3) a more robust model than Eq. (2).

Improved Variance Model Results

To assess the quality of these two formulations, standard dynamic equation averaging procedures are used to calculate the C_4 and C_5 coefficients at certain filter widths [12]. Subfilter variances are then evaluated using each coefficient, and the results are plotted against the best possible result that can be obtained using the model form in Eq. (1). This effectively measures how close the two models come to performing ideally. Figure 2 shows two of these performance plots. The ' $Z_{v,DM}$ ' data represents the C_4 coefficient

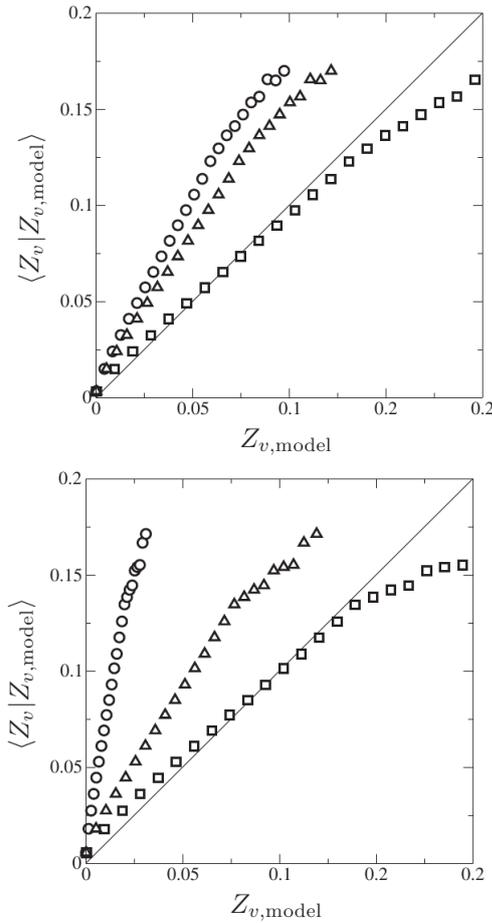


Figure 2: Plot of $\langle Z_v | Z_{v,model} \rangle$ as a function of $Z_{v,model}$. $Z_{v,DM}$ (○), $Z_{v,o2}$ (△), and $Z_{v,LED}$ (□). $y = x$ (—). Left: $\Delta/\eta = 48$, Right: $\Delta/\eta = 64$.

formulation, the ‘ $Z_{v,o2}$ ’ data shows a constant coefficient formulation, and the ‘ $Z_{v,LED}$ ’ shows the C_5 formulation. The large error associated with the dynamic C_4 formulation is due to an important underprediction of the subfilter scalar variance. This underprediction comes from the negative values of C_4 that were observed in the coefficient’s bimodal PDF. The model $Z_{v,o2}$ also underpredicts the subfilter scalar variance because of truncation error [12]. For the C_5 model, there is just a weak overprediction of the high values of the subfilter scalar variance, but for most of the range of the scalar variance, the model is in excellent agreement with the data.

PREMIXED COMBUSTION MODEL FOR LES

In typical large eddy simulations of premixed combustion, flame fronts exist on sub-grid length scales. Consequently, reactive scalar variables cannot be transported accurately. Specifically, the changes in density that occur at the flame front are resolved on only one or two mesh cells. An example for a typical representation of a filtered flame front is shown in Fig. 3. These poorly resolved density changes lead to large numerical errors that affect the solution of all reactive scalar transport equations. The level set, or G -equation, premixed combustion model was proposed for LES in response to this problem [14, 15, 16]. This model, rather than resolving changes through the flame front, tracks, for

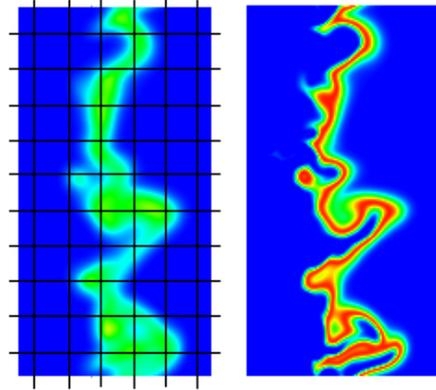


Figure 3: Comparison of a premixed flame front in LES (left) and DNS (right). The color contours indicate the strength of the local chemical source term, and the same scale is used in both plots. A typical LES grid is overlaid on the LES solution, showing that the front appears on only one or two grid cells.

instance, a temperature iso-surface that describes the front.

Since the level set varies smoothly through the flame front, it is well represented on a numerical mesh. However, there are two particular challenges when using level set methods for turbulent premixed combustion in LES. First, the value of the level set away from the flame front has no physical meaning. The typical LES filtering operation can therefore not be applied to the level set function. Instead, a filtering approach needs to be developed that only uses information from the flame surface itself. Second, Pitsch and Duchamp [15] and Pitsch [16] discussed the different turbulence/flame interaction regimes for premixed combustion within the context of LES. In the so called corrugated flamelet regime, the entire flame is thin compared with the smallest turbulent structures. Therefore, in LES, the entire flame thickness is thin compared with the LES filter width. In that regime, the level set will provide an adequate description of the flame. In the thin reaction zones regime, however, the flame is broadened by the turbulence, and although the reaction zone remains thin, the turbulent flame will be broadened over several filter lengths, if the local subfilter Damköhler number is smaller than one. In that case, the knowledge only of the position of a temperature iso-surface is not sufficient for an adequate description of the density changes through the flame. In that regime, the level set solution needs to be complemented with a model for the turbulent flame structure.

Level Set Formulation for LES

The derivation of a level set formulation for LES begins by formulating an equation describing the evolution of a flame front. When a flame front is defined as an isocontour of a progress variable ($C = C_0$), the appropriate equation is produced by multiplying the progress variable transport equation with a delta function,

$$\begin{aligned} & \delta(C - C_0) \left[\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} \right] \\ &= \delta(C - C_0) \left[\frac{1}{\rho} \frac{\partial}{\partial x_j} \left(\rho \mathcal{D}_C \frac{\partial C}{\partial x_j} \right) + \frac{1}{\rho} \dot{\omega}_C \right]. \end{aligned} \quad (4)$$

This delta function can be written equivalently as the derivative of a heaviside function, $\delta(C - C_0) \nabla C = \nabla [H(C - C_0)]$ and can be combined with the other terms

in the transport equation. Some manipulation produces an expression describing the transport of a heaviside function located at the flame front,

$$\frac{\partial[H(C-C_0)]}{\partial t} + u_j \frac{\partial[H(C-C_0)]}{\partial x_j} = D\kappa |\nabla[H(C-C_0)]| + s_{L,C_0} |\nabla[H(C-C_0)]|, \quad (5)$$

where the propagation speed of the C_0 surface, s_{L,C_0} , has been introduced to account for the source terms. Unlike level set formulations, this equation is valid everywhere in space and not just at the flame front surface. This property is important because it means that a standard LES volumetric filter can be applied to the equation. Making the notationally convenient substitution $\mathcal{G} = H(C - C_0)$ and then filtering gives

$$\frac{\partial \bar{\mathcal{G}}}{\partial t} + u_j \frac{\partial \bar{\mathcal{G}}}{\partial x_j} = (\overline{D\kappa})_T |\nabla \bar{\mathcal{G}}| + \bar{s}_{T,C_0} |\nabla \bar{\mathcal{G}}|, \quad (6)$$

where

$$\bar{s}_{T,C_0} |\nabla \bar{\mathcal{G}}| = \overline{s_{L,C_0} |\nabla \mathcal{G}|}, \quad (7)$$

and

$$(\overline{D\kappa})_T |\nabla \bar{\mathcal{G}}| = \overline{D\kappa |\nabla \mathcal{G}|}, \quad (8)$$

represent the introduction of definitions for the filtered burning velocity, \bar{s}_{T,C_0} , and the filtered propagation speed due to curvature, $(\overline{D\kappa})_T$.

Equations (6)-(8) are significant because they can be used, after some further manipulation, to determine the form of the terms that the turbulent burning velocity describes explicitly. Additionally, when both filtering and test filtering are used, they provide the framework for producing a dynamic equation that can be solved to determine the value of turbulent burning velocity model coefficients. For example, since filters commute with temporal derivatives, the application of a broad test filter to Eq. (6) produces a transport equation for $\bar{\bar{\mathcal{G}}}$ (the arrow operator denotes the test filter). If a filter and a test filter instead are applied to Eq. (5) in a single operation, a different form of the $\bar{\mathcal{G}}$ equation is realized. Because these two equations appear in different forms, they can be subtracted from one another to determine an expression relating turbulent burning velocity models associated with different filter widths. This expression can be written,

$$\overline{\left((\overline{D\kappa})_T + \frac{\rho u}{\rho} \bar{s}_{T,u} \right) |\nabla \bar{\mathcal{G}}|} = \left((\overline{D\kappa})_T + \frac{\rho u}{\rho} \bar{s}_{T,u} \right) |\nabla \bar{\bar{\mathcal{G}}}|, \quad (9)$$

where the u subscript denotes that conditioning on the unburned side of the flame front is being considered. Once a specific model for $\bar{s}_{T,u}$ is invoked, Eq. (9) can be solved locally in an LES to determine the value of a coefficient in that model [17].

Flame Structure Model

Level set models are advantageous because they describe flame front propagation at arbitrary mesh resolutions without altering how turbulence affects the front, but they have one inherent drawback. Because a level set represents a 2-D surface, it cannot be used to describe the interior structure of a premixed flame. A field quantity such as a progress variable also must be considered if this interior structure is to be described accurately, but the only way to protect a progress variable equation from numerical errors in premixed combustion is to couple it to a level set at the flame front. In response to this problem, a coupling procedure was

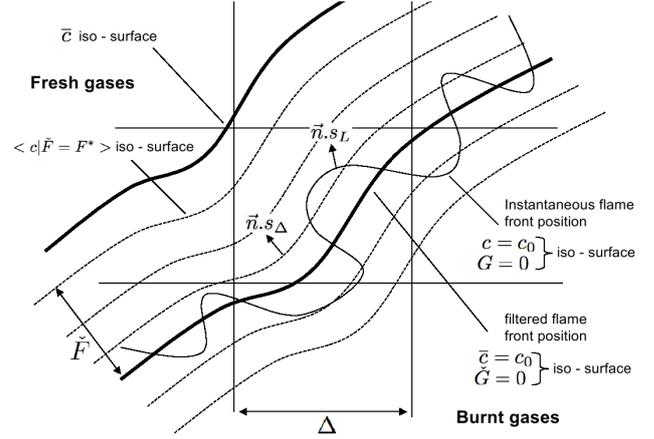


Figure 4: The flame structure model.

developed that can describe 3-D flame structure and account correctly for flame propagation using level sets.

The level set and progress variable coupling is performed by making the source term in a progress variable (\tilde{C}) transport equation dependent on the location of a level set [18]. This dependency is introduced by assuming that the unfiltered C variable can be written as a presumed function of a distance coordinate (F in this context), and that $\dot{\omega}_C$ can be written as a presumed function of C . A 1-D flame structure is assumed additionally, and the $\dot{\omega}_C(C(F))$ function then can be integrated against a filter kernel to find an analytical expression,

$$\bar{\omega}_C(\tilde{C}, \hat{F}, \Delta) = \int_{-\infty}^{\infty} \langle \dot{\omega}_C | \hat{F} = F, \tilde{C} \rangle \bar{P}(F, \mathbf{x}, t, \Delta) dF, \quad (10)$$

where $\langle \dot{\omega}_C | \hat{F} = F, \tilde{C} \rangle$ is the conditional average of $\dot{\omega}_C$ along a surface that is a distance $\hat{F} = F$ away from the filtered flame front position. $\bar{P}(F, \mathbf{x}, t, \Delta)$ is the PDF that describes the likelihood of the location \mathbf{x} being a distance F away from the front. Figure 4 shows a schematic of the new model.

The PDF in Eq. (10) couples the progress variable to the level set and is easy to compute. The conditioned source term in Eq. (10) represents more of a challenge but can be described using a variety of chemical models. This approach leads to excellent predictions of the behavior of a bluff-body-stabilized premixed flame [18]. The flame burns in the thin reaction zones regime, which is an appropriate validation test since, in this regime, turbulence tends to thicken premixed flame structures.

Partially Premixed Turbulent Combustion

Although premixed and non-premixed flamelet solutions can be mapped cheaply and effectively into turbulent flows, these mapping approaches become problematic when partially premixed or multi-regime combustion environments are encountered. In these environments, it becomes unclear whether a premixed, a non-premixed, or an auto-ignition chemical solution should be used to describe chemistry. For example, when fuel is injected into a device by means of a liquid spray, local evaporation and mixing rates might lead to either premixed or non-premixed conditions. Consequently, methods of dealing with multi-regime and partially premixed combustion in flamelet-based LES should be considered.

The flame index proposed by Yamashita *et al.* [19] is one of the only available indicators from the literature that

can be used to determine combustion regimes. The flame index simply examines whether or not gradients of oxidizer and fuel align and then sets the local regime accordingly [19, 20, 21]. This index is based, however, on 1-D geometric arguments, and the extent to which it can be applied to fully 3-D turbulent flames is not yet known. For example, in certain flow settings gradients of fuel and oxidizer do align, but combustion nonetheless remains diffusion-controlled. The flame index does not capture the physics that are relevant in these regimes [21].

Combustion Regime Indicator Formulation.

A new Combustion Regime Indicator (CRI) model has been developed in an effort to capture more of the physics that determine local burning modes. The indicator itself can be derived using a generalized flamelet-type transformation of variables. The mixture fraction, Z , is retained as one of the transformation coordinates because it describes the asymptotic non-premixed regime. The key insight provided by the indicator lies in the second transformation coordinate, which must describe combustion in the asymptotic premixed regime and be statistically independent of Z . A flamelet variable Λ that satisfies these requirements can be defined as the value of the progress variable C that occurs at a stoichiometric mixture fraction ($Z = Z_{st}$) on a given flamelet. When the scalar transport equation for a reacting chemical species is transformed into Z and Λ space, the transformed terms can be grouped according to the asymptotic regime in which they appear. The transformation takes the form

$$\begin{aligned} & (\rho \partial_\tau C + \partial_\Lambda C [\rho \partial_t \Lambda + (\rho \mathbf{u} - \rho_u s_{L,u} \mathbf{n}) \cdot \nabla \Lambda])_1 \\ & + (\partial_\Lambda C [\rho_u s_{L,u} |\nabla \Lambda| - \nabla \cdot (\rho \mathcal{D}_C \nabla \Lambda)] - \rho \frac{\chi_\Lambda}{2} \partial_\Lambda^2 C)_2 \\ & + (-\rho \frac{\chi_Z}{2} \partial_Z^2 C)_3 = \dot{\omega}_C, \end{aligned} \quad (11)$$

where group 1 terms describe unsteady combustion, group 2 terms describe premixed combustion, and group 3 terms describe non-premixed combustion. These terms then can be evaluated in a simulation and compared to one another to determine which asymptotic group of terms balances a local chemical source term. This balance indicates the regime in which a flame burns.

A generalized model for partially premixed combustion can therefore be formulated on the basis of the coupled level set/reaction progress variable approach using the combustion regime indicator. Depending on the value of the combustion regime indicator, closure of the reaction progress variable comes either from the non-premixed tables, in which case the formulation locally reduces to the non-premixed FPV model, or from a combination of premixed chemistry tables and the level set solution, in which case the premixed combustion model is recovered.

Model Application: LES of a Low Swirl Burner.

The CRI-based combustion model for partially premixed combustion is tested in an LES of the low swirl burner shown in Fig. 5. This burner has been the subject of previous experimental and computational investigations [24, 23, 25] and is particularly interesting to investigate from the standpoint of regime prediction. Regime predictions are interesting because the coflowing air in the burner mixes with the primary premixed fuel stream and changes the nature of the combustion regime along the downstream direction. Figure 5 shows two images from the LES, in which the CRI has been used actively to apply asymptotic combustion solutions [26]. In particular, the bottom plot indicates how the coflowing

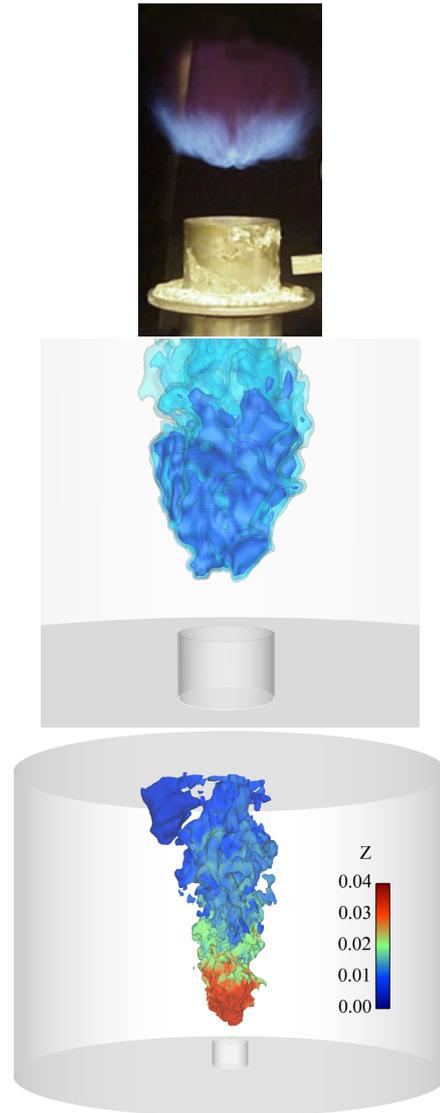


Figure 5: Instantaneous fields from the swirl burner. Left: Typical LSB experimental image, from Cheng [22, 23]; Middle: Three \tilde{C} isocontours from the LES; Right: LES level set representation of the flame front, colored by \tilde{Z} ;

air leans out the primary fuel stream. The level set isocontour that is shown in this plot is colored by mixture fraction, which steadily decreases between the nozzle and the burner exit. The upper two plots in this figure show that the flame predicted by the CRI methodology instantaneously compares well to a typical experimental visualization of the burner.

Figure 6 shows time-averaged profiles from the centerline of the burner. The mean axial velocity is shown along with the mean and rms temperatures as a function of the burner axial coordinate. This figure is particularly noteworthy because it demonstrates that the central flow feature of the swirl burner is captured accurately by the LES. This feature is the linearly decreasing centerline axial velocity profile. The decrease in axial velocity is created by the recirculation region that the swirling flow sets up. The decreasing velocity profile acts to stabilize the position of the burner's premixed flame. The figure shows that the LES temperature profiles are in especially good agreement with the experiments. The

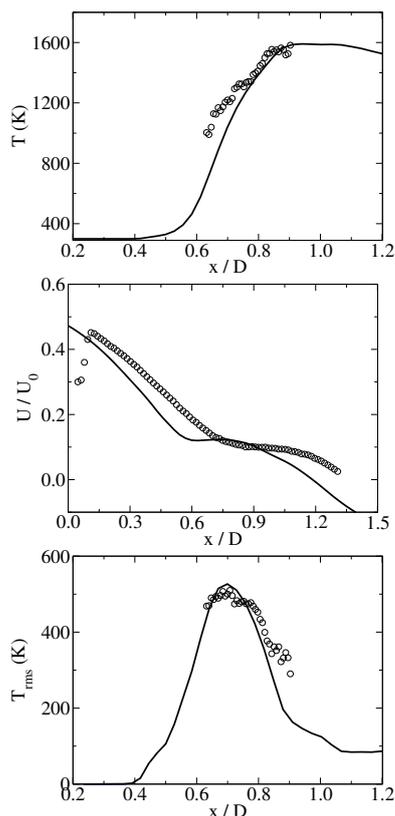


Figure 6: Time averaged swirl burner centerline profiles. LES solutions (—); Experimentally measured profiles (ooo) [25]. Axial velocity, axial RMS velocity, temperature, and RMS temperature are shown as a function of downstream displacement along the burner centerline.

agreement suggests that the combustion model is performing well, and that the CRI and generalized flamelet transformation theory can be applied consistently in LES.

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