 The Open Thermodynamics Journal, 2010, *4,* 76-85

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Large-Eddy Simulation for Combustion Systems: Modeling Approaches for Partially Premixed Flows

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Abstract: Combustion models often appear in forms that are customized for specific applications. This process of customization produces modeling approaches that tend to be very different from one another in terms of cost, accuracy, and applicability. For example, many combustion models have been developed to describe either the asymptotic premixed or the asymptotic non-premixed combustion limit. These idealized regimes are chosen as the basis for modeling approaches because the associated combustion physics are understood sufficiently well to be cast in a framework that accounts for how turbulence and chemistry interact. Partially premixed regimes and regimes that involve transitions between premixed and non-premixed behavior, however, are not very well understood. Consequently, most readily available modeling approaches do not account for these mixed regimes in a very careful fashion. This presents a particular challenge to further model development, since these partially premixed and transition processes are very important in realistic combustion devices. In this review, the particular challenges associated with modeling partially premixed combustion in LES will be discussed and the applicability of common LES combustion models to partially premixed processes will be assessed.

Keywords: Large-eddy simulation, partially premixed combustion, combustion modeling.

1. INTRODUCTION

Persistent and focused scientific efforts have led to a relatively accurate and broadly accepted understanding of many of the fundamental physics behind combustion processes [1-5]. In spite of this understanding, however, the task of developing predictive computational tools that can describe how particular combustion events evolve has remained extremely challenging [4-6]. This challenge is the subject of continuing study because predictive computational tools will be needed if combustion-based engines are ever to be truly optimized. More specifically, engine performance metrics such as efficiency, robustness, noise, and cost are all non-linearly sensitive to the details of the combustion process.

Many of the presently available tools that have been designed to simulate combustion devices rely on a certain amount of empiricism [3,5,7,8]. When considering questions that relate to low order design concerns, this empiricism is warranted and can be very useful. For example, a combustion model that simply differentiates between burned and unburned gas, and that captures the corresponding density change, may provide a great deal of insight into an engineering application. When more detailed considerations such as pollutant production, flame stability, or robustness are considered, however, a greater demand is placed on a model. For these metrics, even a small degree of empiricism can lead to large errors and inappropriate design estimates. To deal with these detailed considerations, models that can account for a wide variety of fundamental physics must be employed. Computational tools such as large eddy simulation (LES) provide a platform for leveraging these models, and the application of LES is continuously becoming more widespread. The issue of model accuracy, however, continues to influence the extent to which industry can rely of many of these calculations.

The multi-disciplinary, multi-physics nature of simulating an engine chamber significantly increases the challenge of predicting its behavior. Between fuel injection and exhaust removal, for example, processes that may be observed include liquid jet injection, primary jet atomization, secondary droplet atomization, spray evaporation, chemistry and turbulence interaction, radiation, soot particulate formation and interaction, and the evolution of chemistry over very wide ranging time scales. Pollutant formation is an example of this last kind of process, and pollutants will of course evolve as a function of all other physical processes. An empirical model for dealing with primary atomization may accordingly cascade through these processes and introduce an error in the amount of predicted NO_X coming from an engine.

Because of these multi-physics challenges, the field of combustion modeling can be said to encompass a variety of branches. These branches include the topics of chemistry reduction for use in computations [9], multiphase modeling [10], pure turbulence modeling [11], asymptotic combustion regime analysis [2], and turbulence-chemistry interaction [2-3,5].

This last branch, turbulence-chemistry interaction, has occupied a central place in the field for some time. Yet it still presents one of the greatest challenges to the further advancement of the field. This is partly due to the particularly important non-linearity that is inherent in both combustion and turbulence, and to the detailed nature of the processes that contribute to their interaction. Although some difficulty in forming predictions of turbulence and chemistry interac-

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1874-396X/10

tion is to be expected, it has, again, meant that practical simulations have been limited by the empiricism of the models being employed.

In recent years, combustion modeling has been moving toward the idea that tractable approaches can in fact be based on fundamental physics, with only a minimal involvement of user-tuned-parameters. Several models, for example, now employ detailed chemical mechanisms and yet are designed to function in the context of LES codes for complex geometry, multi-physics combustors.

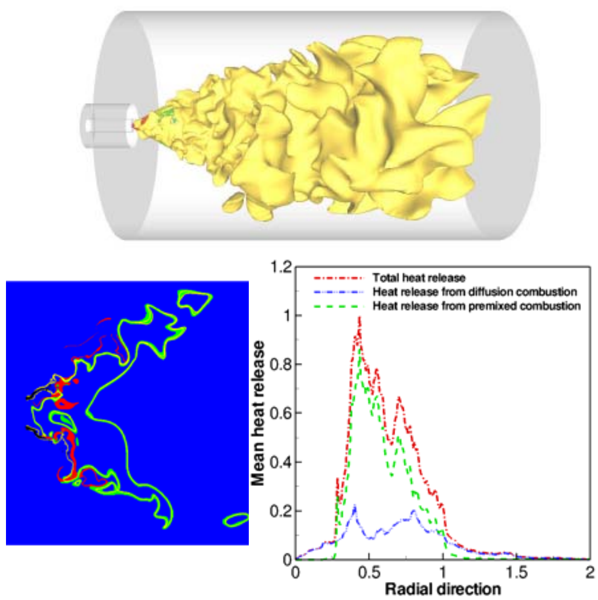

Fig. (1). DNS of a spray combustor from Ref. [12]. Top: Temperature isocontour in the combustor. Bottom Left: Flame index in combustor cut plane (see section 3.5), with red representing premixed and green representing non-premixed combustion. Bottom Right: Azimuthally integrated premixed, non-premixed, and total heat release in a cross section of the domain. Heat release is normalized by its maximum value, and the radial coordinate is normalized by the inlet pipe diameter.

A representative simulation that has been designed to examine turbulence and chemistry interactions for the purpose of model development is presented in Fig. (**1**). This simulation is a DNS of a spray combustor with co-flowing and swirling gas inlets [12]. The combustor geometry is shown in the upper plot in the figure, and the Reynolds number based on the gas inflow velocity and the outer inlet pipe diameter is Re=2000. Traditionally, a spray combustor such as this would be treated as an example of non-premixed combustion, and it would be assumed that flame structures align with gradients in the mixture fraction field variable. An interesting result of this simulation, however, is that the combined effects of spray injection, evaporation, and turbulent mixing actually lead to a great deal of premixed-type behavior. For example, an instantaneous plot of the flame index (reviewed in section 3.5) is shown in the lower left of Fig. (**1**), and an azimuthally averaged plot of heat release at a combustor cross section is shown in the lower right. These figures demonstrate that premixed combustion readily appears at locations slightly downstream of the spray injection point, and that premixed behavior can be responsible for the majority of the heat release at such locations. This simulation helps to motivate the present review. In multi-physics simulations of modern combustors, multiple combustion regimes can be expected. Moreover, these regimes can appear separately in distinct flow regions, or blend together to produce truly partially premixed behavior.

2. THE FRAMEWORK BEHIND PARTIALLY PREMIXED MODELING IDEAS

In this section, a brief discussion of how partially premixed combustion tends to appear in flows is given. A step back is then taken, and the ideas that have led to modern single regime modeling approaches are considered. A consideration of single regime ideas is important since present combustion models tend not to be targeted for the partially premixed regime. Rather, traditional single regime models underpin the formulations of many current attempts to deal with mixed regimes.

2.1. Partially Premixed Combustion's Role in Flame Stabilization

Operational stability is the most important requirement for any combustor. Flame stabilization processes that ensure this requirement is met can be broadly organized into several categories [2,13,14]. Often the processes in these categories work in conjunction with one another within a device. The physics behind the categories frequently lead to mixed-regime or partially premixed behavior.

Flame stabilization processes may be very roughly organized as 1) aerodynamic in nature, 2) propagative in nature, 3) dependent on auto-ignition, or 4) dependent on an external ignition source. In aerodynamic stabilization, for example, integral scale fluid mechanics are of first order importance, and the flow field continuously transports heat or reactants to the flame. The aerodynamic mechanism is often established through a recirculation zone set up by a bluff body or swirler [7,15]. Flame propagation is a second stabilization mechanism that often appears in combination with other mechanisms. Premixed burning may provide a stabilizing influence, for example, in the center of a recirculation zone or in a lifted jet flame configuration [9]. Auto-ignition processes that form the third mechanism can occur under a wide variety of conditions. Preheating, mixing, and pressure are all particularly important in establishing this mechanism. Examples for this mode can be found in scram-jet combustion and aircraft engine afterburners. The fourth mechanism, external stabilization, is most often enforced through the use of a spark plug, such as in a gasoline engine. Another example of this mechanism would be plasma based flow control.

These four flame stabilization mechanisms will often produce mixed-regime combustion. In a typical aerodynamic stabilization, for example, burned combustion products are recirculated and mix with cold, segregated fuel and air streams [7,15]. The hot combustion products may preheat portions of either the fuel or air streams and thus push the system away from a pure non-premixed asymptote and toward an unsteady asymptote. Conversely, if a turbulence event causes the recirculation of hot products to be delayed, the fuel and air streams may mix at a cold temperature. The system is then pushed toward a premixed asymptote.

Because the flame propagation and auto-ignition mechanisms often occur in the presence of stratification, they tend to display partially premixed characteristics. Compression ignition in diesel or HCCI engines occurs after an initial spray injection has evaporated. Depending on the particular ignition timing, the evaporation process can lead to pockets of gas with various degrees of premixing. Partially premixed combustion must therefore be considered in addition to auto-ignition.

2.2. The Balance of Transport and Chemistry in Combustion Processes

Most of the current approaches to dealing with partially premixed combustion in LES are rooted in traditional modeling ideas that do not consider mixed regime asymptotics. Rather, these approaches often draw heavily on concepts developed for pure non-premixed or pure premixed LES combustion modeling. The LES ideas, in turn, draw on RANS ideas. In the area of non-premixed combustion, this development process has been somewhat linear, since the mixture fraction variable is as useful for describing combustion in LES as it is for describing it in RANS. The increased information that is available in LES is easy to correctly leverage in mixture fraction based models. Specifically, critically important balances between transport and chemistry can be captured as a function of mixture fraction in the purely non-premixed regime. Increased resolution of the mixture fraction variable directly translates into improved predictions, since fluctuations in this variable correspond very well to fluctuations in the combustion process. This advantage of the mixture fraction variable is expected to remain relevant in partially premixed settings.

In the premixed regime a somewhat different situation exists. The progress variable is the important chemistry parameterization coordinate, and it too can be used to map a small-scale balance between chemistry and turbulence into a flow solution. Unlike the mixture fraction variable, however, the progress variable (as well as many other reactive variables) tends to transition between unburned and burned values over only a few mesh points in premixed LES. Said more precisely, the filtered flame thickness is often on the order of the filter size, which in LES typically corresponds to the mesh spacing. RANS approaches, where ensemble averaging broadens the mean flame, and where resolution constraints are therefore less of an issue, do not always map as easily into LES. This does not imply that premixed RANS models are any more descriptive than premixed LES models. Rather, it implies that the unique characteristics of LES must be carefully considered if reactive fronts are to be accounted for in this technique.

This particular issue for premixed LES can be illustrated using the premixed combustion LES regime diagram shown in Fig. (**2**) [16]. The diagram parameterizes how turbulence and chemistry can interact in a premixed LES. On the vertical axis the ratio of the LES filter width Δ and the flame thickness l_F is used as a parameterizing coordinate. On the horizontal axis the Karlovitz number, Ka, is used for parameterization. Ka is the ratio of the chemical time scale and the smallest flow time scale. Other variables in the figure include the Gibson scale l_G, describing the minimum size of eddies that can interact with the flame front, the Kolmogorov scale η, the width of the flame inner reaction zone δ, the Damköhler number Da, and the Reynolds number associated with the filter width, Re_Δ.

The l_m variable in this diagram represents the length scale associated with the turbulent flame thickness, and the $l_m=\Delta$ line passes directly through the thin reaction zones regime. This means that a large variety of flame structures in the thin reaction zones and corrugated flamelets regime are smaller than the filter size and are left unresolved. Beyond this issue of resolution, a premixed flame's location within the regime diagram will significantly influence the speed at which the filtered flame propagates. These particular challenges must be dealt with when modeling turbulent premixed combustion in LES, and will have to be considered in partially premixed approaches as well.

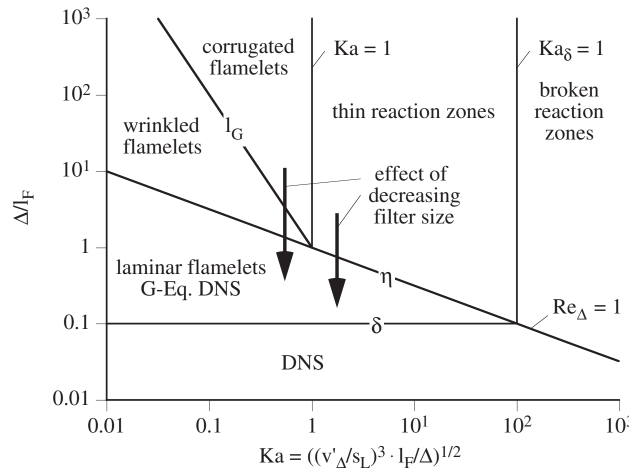

Fig. (2). Premixed regime diagram for LES, from ref. [16].

In closing this section, it is important to again emphasize that the single regime combustion ideas presented here form the basis of many partially premixed approaches. Models that are solely designed to capture partially premixed transport and chemistry interactions are not readily available.

3. MODELING APPROACHES FOR LES OF PARTIALLY PREMIXED COMBUSTION

As discussed in section 1, a gap has historically separated the level of physical detail that is considered in fundamental canonical combustion studies, and the level of physical detail that is considered in engineering models of realistic devices. Due to the increasing availability of computational resources, and to the resulting increase of massively parallel LES simulations, however, this gap is diminishing. Moreover, a wide variety of models for describing unresolved turbulence and chemistry interactions are being continuously developed in an attempt to close this gap completely. For LES, a list of these models would include thickened flame approaches, linear eddy models, conditional moment closure, transported FDF approaches, and flamelet models. Presently, though, empirical influences linger in many of these models. In the following sections, the models will be analyzed in the context of partially premixed combustion, where the gap between the approaches being used and the fundamental governing physics may be the widest.

3.1. Thickened Flame Models

Thickened flame models for LES [17-22] solve transport equations for chemical species, and use Arrhenius rate expressions to describe species' reactions. These transport equations can be solved, however, only when flame structures are adequately resolved. Since resolving realistic flame structures is not affordable in LES, thickened flame models artificially broaden flame structures to ensure convergence of the species equations.

The artificial flame broadening is accomplished by multiplying the diffusive terms in the scalar transport equations by a thickening factor, F, that may be as large as ten or twenty. The reactive source terms are divided by the same factor. An unfiltered transport equation for a reactive species ϕ_k may then be written [17-18]

$$\frac{\partial}{\partial t}\left(\rho\phi_k\right) + \frac{\partial}{\partial x_j}\left(\rho u_j \phi_k\right) = \frac{\partial}{\partial x_j}\left(\rho F \mathcal{D}_k \frac{\partial}{\partial x_j}(\phi_k)\right) + \frac{\rho\dot{\omega}_k}{F}, \quad (1)$$

where the chemical source term $\dot{\omega}_k$ is evaluated using an Arrhenius-type expression, u_j is the flow velocity in the jth direction, ρ is the density, and D_k is the species diffusivity. The flame thickening in this equation has important implications for combustion modeling. For example, the thickening creates the need for an empirical efficiency function that compensates for the model's effect on the turbulent flame propagation speed. Specifically, the increase of the diffusion coefficient and the decrease of the chemical source term lead to an increase in the Karlovitz number by a factor of F. The sub-filter Damköhler number, which is related to the quantity l_m/Δ from Fig. (**2**), is also changed by a factor of $1/F$. In the combustion regime diagram in Fig. (**2**), therefore, the model moves the computed regime to the lower right.

In the context of partially premixed combustion, the thickened flame approach can be viewed from two perspectives. One perspective, for example, would be that the approach is regime independent. This perspective would stem from the idea that no information about flame asymptotics is required in the implementation. It would suggest that the approach is very general, and it has indeed been applied in a variety of simulations where partially premixed combustion would be expected. These applications include helicopter engine combustors [19], partially premixed swirl burners [20], and industrial gas turbines [21]. Results that agree well with experimentally measured velocities, temperatures, and pressure fluctuations have been obtained in each of these cases. A mesh refinement study has also shown that the approach produces reasonably mesh independent results [22]. The exception to this mesh-independence is the scalar variance, which is known to be important in the context of combustion LES.

A second perspective, however, would be that this approach changes the nature of turbulence and chemistry interactions by reducing the time scale for transport and increasing the time scale for chemistry. When the Karlovitz number in a flame is of order ten or larger, for example, the model may move the computed flame into the broken reaction zones regime. It might then exhibit local extinction, which the actual flame would not encounter. Furthermore, the increased diffusivity in Eq. **1** will affect how the model characterizes non-premixed quenching processes. Typically, a non-premixed flame will extinguish when the local scalar dissipation rate χ increases beyond some critical value. The factor F will change the computed value of this critical dissipation rate, and may cause quenching to be incorrectly predicted.

Finally, the model neglects the small-scale interaction between transport and chemistry that characterizes both the non-premixed and the premixed regimes. Since these regimes are not correctly characterized, it would not be expected for the even more complex partially premixed regime to be well characterized. This second perspective, then, emphasizes the idea that small-scale transport and chemistry processes are critically important, and that altering the associated time scales leads to significant errors in predictions.

In considering these perspectives, it is interesting to note that most thickened flame implementations employ only one- or two-step chemistry, presumably to minimize the appearance of even smaller scale inner flame layers. In the limit of these low-order chemical mechanisms, the differences between premixed and non-premixed flame structures tend to disappear [23]. Consequently, combustion events that occur in differing regimes may not behave differently in the current implementations of the thickened flame approach. Moreover, partially premixed combustion may not appear as a distinct phenomenon in the implementations.

It is possible that the undifferentiated descriptions of sub-filter premixed and non-premixed physics in the thickened flame model do not significantly affect global flow statistics such as mean temperature. This could be argued on the grounds that the value of the burned and the unburned densities in the model are correct regardless of the regime, and that these densities are the quantities of first order importance. The neglect of small-scale transport and chemistry considerations may, however, strongly affect other results such as pollutant and soot formation. These secondary quantities tend to be more sensitive to regime dependent flame structures than equilibrium quantities. It appears that further simulations and testing are needed if the extent of the thickened flame approach's applicability to minor species and pollutant predictions is to be fully mapped.

3.2. Linear Eddy Models (LEM)

Linear Eddy Models (LEMs) attempt to explicitly solve for a reduced representation of subfilter turbulence/chemistry interaction [24-33]. Within every LES cell, LEM models create a 1-D mesh on which a subfilter transport equation is solved

$$\rho\left(\phi_k^{*,n+1} - \phi_k^n\right) = \int_t^{t+\Delta t_{\mathrm{LES}}} \left[F_{mix} + \frac{\partial}{\partial x}\left(\rho\mathcal{D}_k\frac{\partial}{\partial x}(\phi_k)\right) + \rho\dot{\omega}_k\right] dt, \quad (2)$$

where

$$\phi_k^{*,n+1} - \phi_k^n \quad (3)$$

is the local subfilter contribution to a scalar field's evolution, F_{mix} describes subfilter convection, and Δt_{LES} is a global LES time step. The 1-D mesh typically consists of more than 10 mesh points [7,25], and in addition to the approximations it implicitly represents, the subfilter convective term F_{mix} must be modeled. This is accomplished using a triplet mapping procedure that stochastically rearranges the 1-D scalar fields using specified frequencies and lengths. For example, a stirring frequency λ which determines how often data on the 1-D mesh is stochastically rearranged is modeled as [7]

$$\lambda = \frac{54}{5} \cdot \frac{\nu \mathrm{Re}_\Delta}{C_\lambda \Delta^3} \cdot \frac{[(\Delta/\eta)^{5/3} - 1]}{[1 - (\eta/\Delta)^{4/3}]}, \tag{4}$$

where C_λ is a constant, Re_Δ is a Reynolds number associated with the filter scale Δ, η is the estimated Kolmogorov length scale, and ν is the viscosity. Arrhenius rates are used to describe the subfilter chemical source terms, and once the 1-D solutions have been solved, they can be Favre filtered to convey subfilter information to the flow solver mesh.

Just as with thickened flame models, one of the particular advantages of LEM models is that they do not require *a priori* assumptions about the burning regime. Unlike thickened flame models, however, the 1-D subfilter meshes are capable of resolving and accounting for how transport and chemistry balance on the smallest scales. The LEM model therefore has the advantage of representing the multi-scale nature of combustion processes.

With respect to partially premixed combustion, it is interesting to note that these subfilter meshes are only capable of moving information in one direction. For example, in a given cell a subfilter mesh could capture a non-premixed flame associated with a gradient of mixture fraction. It could also capture a premixed flame associated with relatively constant mixture fraction. Collocated gradients of mixture fraction and progress variable, however, can apparently be captured only to the extent they both exist in the direction of the 1-D mesh.

In spite of its ability to capture the coupling between diffusion and reaction on the small scales, quantities such as the stirring frequency in the model are empirically determined. While this empiricism has resulted in good agreement with experimental predictions in realistic combustor settings [7], its performance has not yet been fully characterized. Additionally, because chemistry is locally and explicitly solved for, LEM models for combustion can be relatively costly. Patel *et al*. [7] report, for example, that the introduction of an LEM combustion model using a three-step chemical mechanism increased the cost of solving an LES of a combustor by a factor of 10 relative to the non-reacting case. Due to this cost, relatively simple (2 or 3 step) chemical mechanisms may need to be employed. The extent to which this chemistry can capture the details of pollutant or soot production in a partially premixed flame is, like in the case of the thickened flame model, not yet fully known.

3.3. Conditional Moment Closure Models

Conditional Moment Closure (CMC) approaches [34-40] attempt to describe chemistry by solving for values of chemical species that have been conditioned on a particularly relevant scalar. A mixture fraction or progress variable is typically used for this purpose. In LES, density weighted filtered conditional moments of the scalar ϕ_k may be written [36]

$$\widetilde{\phi_k|\eta}(t, \mathbf{x}, \eta) = \frac{\int_V \rho \cdot \phi_k \cdot \delta(\xi - \eta) \cdot G(\Delta)\, d\mathbf{r}}{\int_V \rho \cdot \delta(\xi - \eta) \cdot G(\Delta)\, d\mathbf{r}}, \tag{5}$$

where here η is the sample space variable associated with the conditioning scalar, ξ is the local value of that scalar in the flow field, δ represents a standard delta-function, $G(\Delta)$ is the LES filter, and V is the physical domain. A transport equation for this quantity can be derived [36], but it contains a variety of unclosed terms.

In traditional CMC, the conditioning scalar quantity must be treated as an independent coordinate in a simulation. In single regime combustion LES, this would mean that a typical mesh is extended from three dimensions spanning Cartesian space to four dimensions that span a scalar space in addition to Cartesian space. The problem when dealing with partially premixed combustion is immediately apparent: a fully coupled conditional dependence on progress variable and mixture fraction would require an untenably large five dimensional mesh. It would be possible to simplify this constraint and consider an uncoupled progress variable and mixture fraction dependence in which cross derivatives of the conditioning scalars are neglected. This might correspond to considering separate, uncoupled premixed and non-premixed asymptotic limits. This kind of a simplification for partially premixed regimes, however, still represents a significant cost increase relative to a single regime CMC.

An approach that is closely related to CMC is Conditional Source term Estimation (CSE) [38, 39]. In this approach, independent variables are not added to the problem's dimensionality or to the computational mesh. Rather, functions describing the conditional scalar profiles are determined by inverting a system of equations relating the conditional profiles to filtered or mean values of a set of scalars [38, 39]. This approach requires solving transport equations for several reactive quantities, so that there are an adequate number of mean or filtered scalar values to accomplish the inversion at a given mesh point. Flamelet-like asymptotic chemistry solutions are also used in the inversion process to combat the ill-conditioned nature of the problem. As noted by the CSE developers, however, the use of these flamelet solutions allows a somewhat more general chemistry/flow interaction to be considered than with purely steady flamelets [38]. The unsteadiness that can be accounted for may be helpful in partially premixed settings.

If CSE were to be employed for partially premixed modeling, the nature of the inversion could grow considerably more complex due to the conditioning on progress variable as well as mixture fraction. Furthermore, separate premixed and non-premixed solutions might need to be used to deal with the ill conditioning along the separate directions. It is not yet foreseeable that a truly partially premixed asymptote could be used to facilitate inversion, since such asymptotes remain unavailable despite persistent efforts in the flamelet community.

Another consideration of importance in a CSE method for partially premixed combustion LES is the issue of flame structure resolution. Reactive scalar equations need to be transported in these methods, but numerical errors are likely to contaminate these solutions if they are solved using traditional transport schemes. This is similar to the numerical issue that arises when a progress variable or reactive species is solved in an LES of a premixed flame.

3.4. Transported FDF Models

Transported FDF models for LES (and PDF models for RANS) [41-45] attempt to describe chemical reactions by explicitly solving for subfilter distribution functions. FDF approaches [8,44] use a transport equation for the filtered density function (FDF) as a starting point

$$\frac{\partial}{\partial t}(\mathbf{F}_L) + \frac{\partial}{\partial x_j}(\widetilde{u}_j \mathbf{F}_L) + \frac{\partial}{\partial x_j}(\widetilde{u_j'|\psi_i \mathbf{F}_L}) = -\frac{\partial}{\partial \psi_m}\left[\left(\frac{1}{\overline{\rho}}\overline{\frac{\partial}{\partial x_j}\left(\rho \mathcal{D} \frac{\partial}{\partial x_j}\phi_m\right)|\psi_i} + \mathbf{S}(\psi_m)\right)\mathbf{F}_L\right], \tag{6}$$

where $\mathbf{F}_L$ is the FDF itself, $\mathbf{S}(\psi_m)$ is the source term which depends on all chemical species ψ_m, and ψ_i describes the local values of those species. $\mathbf{F}_L$ is a vector quantity, and each vector element is in turn a function of a sample space that describes the likelihood of finding a particular density weighted value of a chemical species. Consequently, the integration of $\mathbf{F}_L$ against the sample space variables completely characterizes the subfilter field.

Because Eq. (**6**) is computationally intractable, alternative solution techniques are used to describe the evolution of the FDF. These techniques track chemistry realizations in either a Lagrangian or Eulerian sense, often with the realizations formulated as particles. The greatest challenge associated with this technique is to model the conditional diffusion, or mixing, term that appears in Eq. (**6**) [8,41]. If a very accurate mixing model were in place, transported FDF approaches would be able to fully characterize partially premixed combustion, regardless of whether or not the typical mixture fraction and progress variable coordinates are aligned in any way. Indeed, the approach would then be fully closed and would not be subject to any *a priori* assumptions about the regime.

Although the transported FDF approach is therefore very promising and powerful, the difficulties associated with describing mixing temper its current applicability. The models that are presently used for the mixing term are somewhat empirical [8], and do not always predict how the small-scale balance between reaction and transport is struck. This balance is especially important in premixed flames. In the context of RANS, for example, transported PDF methods are capable of agreeing well with experiments for certain values of tunable mixing model coefficients [45]. The agreement, however, can significantly deteriorate if the mixing model coefficient is adjusted [45]. It appears that limited work is available regarding the corresponding sensitivity for premixed combustion LES.

This difficulty with the premixed limit is expected to extend to partially premixed regimes. It may be possible to argue that the advantages of fully closed chemical source terms and detailed chemistry outweigh the inaccuracies of the mixing model in partially premixed flows. Conversely, errors in the description of mixing in a flow may overwhelm any advantages gained by the access to many chemistry realizations. This question regarding where the dominant error in an approach appears is, by this point, clearly an important theme in the discussion of partially premixed combustion. Just as for the previously discussed models, further comparisons to DNS and experiments are needed to formulate answers.

3.5. Flamelet Models

Flamelet models are the final LES combustion approach that will be considered. These models attempt to describe the subfilter evolution of chemistry by mapping combinations of 1-D pre-computed asymptotic flame solutions into a 3-D flow field. The well known 1-D auto-ignition, steady non-premixed, and steady premixed flame equations are

$$\begin{aligned} \rho\frac{\partial}{\partial t}(\phi_k) &= \rho\dot{\omega}_k, \\ -\frac{\rho}{2}\chi_Z\frac{\partial^2}{\partial Z^2}(\phi_k) &= \rho\dot{\omega}_k, \\ \rho_u s_{L,u}\frac{\partial}{\partial x}(\phi_k) - \frac{\partial}{\partial x}\left(\rho\mathcal{D}_k\frac{\partial}{\partial x}(\phi_k)\right) &= \rho\dot{\omega}_k, \end{aligned} \tag{7}$$

where Z is the mixture fraction coordinate, χ_Z is the scalar dissipation rate, and $s_{L,u}$ is the premixed laminar burning velocity. The process of mapping the solutions of these equations into an LES typically involves convoluting them with a PDF whose shape is presumed. A variety of approaches to doing this for both non-premixed and premixed combustion exist [5], including Flamelet Prolongation of ILDM (FPI) [46], Flamelet Generated Manifolds (FGM) [47], the Flamelet Progress Variable (FPV) approach [48,49], unsteady or Lagrangian flamelets, level set methods [50,51], and the Flame Surface Density (FSD) approach [52,53].

Three advantages of the flamelet model have led to its relatively widespread consideration and study. These advantages include the method's minimal computational cost, the method's ability to consider arbitrarily detailed chemistry in the flamelet space, and the method's multi-scale nature that is based on the correct prediction of the balance that exists between chemistry and transport on the smallest scales. In the context of partially premixed combustion, the first two of these advantages remain, but a caveat must presently be associated with the third advantage. This caveat will be discussed below.

The first question that might be considered in the development of a flamelet approach to partially premixed combustion is whether a useful partially premixed asymptotic equation set can be formulated or derived. A similar mixed regime equation has been derived and applied successfully, for example, in the form of the unsteady flamelet equations that represent both auto-ignition and non-premixed combustion. With regards to the partially premixed regime, however, several physical constraints suggest that such a derivation will not be tractable in the immediate future.

For example, the statistical dependence of the mixture fraction variable and the progress variable implies that these quantities cannot be simultaneously used as basis coordinates in a transformed, 2-D flamelet space. The partial differentiation operators that are expanded in the transformation process do not allow for such interdependence. This first issue of statistical dependence can be eliminated, however, by defining a reaction progress parameter, Λ, in place of the progress variable [23,49]. Λ represents the value of the progress variable at a single point on a non-premixed flamelet and is therefore independent of the mixture fraction Z. Taking partial derivatives with respect to both Z and Λ is then tractable. Λ is not conserved, however, and an associated source term appears in the 2-D transformed flamelet equation set. This source term causes the transformed equations to be somewhat more complex than typical flamelet equations [23,49]. Because of complications such as these, no flamelet type equation for a partially premixed regime has yet been widely considered.

Consequently, extensions of the flamelet approach to partially premixed regimes have largely focused on methods of merging the readily available premixed and non-premixed asymptotic solutions. This merging represents the caveat that must be associated with a flamelet model's ability to capture the balance between transport and chemistry. In the partially premixed limit, flamelet models tend to represent this balance through contributions from two discrete regimes, whereas in the actual flow the cross terms through which the regimes interact certainly can be of importance. At this point, the error associated with using two discrete regimes to represent a partially premixed process is not well understood. In many important engineering flows, however, relatively distinct regions of non-premixed and premixed combustion can be identified, and approaches making use of premixed and non-premixed regimes would undoubtedly be capable of capturing this behavior if formulated correctly. Moreover, it is reasonable to conjecture that an appropriately diverse ensemble of flamelets, combined correctly, could describe certain aspects of mixed regime combustion. With these ideas in mind, partially premixed flamelet modeling has proceeded forward with the development of implementations that integrate multiple asymptotic limits.

A variety of issues concerning how these multiple asymptotic limits should be mapped into a flow field must be considered if combined regime methods are to be successful. One of the more developed approaches to dealing with these issues employs the so-called flame index [46,54-56]. This index, ζ, is defined using information about the gradients of the fuel mass fraction Y_F and the oxidizer mass fraction Y_O,

$$\zeta = \frac{\nabla Y_O \cdot \nabla Y_F}{|\nabla Y_O|\,|\nabla Y_F|}. \tag{8}$$

The regime is said to be premixed when these gradients align, and is said to be non-premixed if the gradients do not align. A filtered formulation of this index has been developed for LES, and this approach includes a subfilter closure component [54]. This indicator is advantageous in that it is straightforward to implement. Oxidizer and fuel mass fractions, for example, are usually readily available from a tabulated flamelet solution database. The disadvantage of this indicator is that it does not examine the underlying physical processes that contribute to the flame structures associated with each regime. As such, it incorrectly predicts the regime under certain mixing conditions, and may require modification [46].

A second approach to regime mapping has been developed in an effort to more closely determine the relative importance of transport and chemistry. This second approach can be referred to as the combustion regime index. Rather than use geometrical gradient information, it starts from a scalar transport equation in which the coordinate basis has been transformed from Cartesian space to Z and Λ space [23]. Such a flamelet transformation was earlier described as being difficult to solve. The terms that appear in the transformed equation, however, can each be associated with a particular regime, and then evaluated in the limits of those regimes using standard flamelet solutions. The terms can then be compared with one another at each mesh location in a simulation. At a given location, the largest of the terms must balance the majority of the chemical source term. This approach therefore argues that the regime associated with the terms that balance the chemical source indicates the dominant regime in the flow field. In analogy to a typical analysis of a turbulent kinetic energy equation, this second mapping approach effectively examines the term-by-term budget of the flamelet transformation to determine which limiting set of terms is most important. The resulting regime index Θ that this approach considers may be written to leading order as [9]

$$\Theta = \frac{\partial_\Lambda C\left[\rho_u s_{L,u}\,|\nabla\Lambda| - \nabla\cdot(\rho\mathcal{D}\nabla\Lambda)\right]}{-\rho\frac{\chi_Z}{2}\partial_Z^2 C}, \tag{9}$$

where the variable definitions from Eq. **7** still hold, and the premixed-type terms appear in the numerator and the non-premixed-type terms appear in the denominator. A filtered form of this indicator can readily be written for LES.

Regime mapping approaches that use a flame index or a combustion regime index have been successfully applied in LES computations [23,54]. Additionally, a good agreement with experimental results was obtained when the combustion regime index was applied to the simulation of a swirl burner consisting of a primary premixed stream sheathed in a coflow of pure air [23]. As with all of the models that have been discussed, however, further testing, simulation, and validation efforts are needed before the influence of the partially premixed regime mapping can be definitively isolated and quantified.

Finally, it should again be noted that in flamelet LES approaches where multi-regime mapping occurs, a transport equation for the progress variable must be solved. Due to the resolution constraints associated with premixed LES, special methods are required to ensure the progress variable equation propagates at the correct turbulent flame speed in premixed regimes. In the context of flamelet models, level set methods are one of the only techniques presently being used for this purpose [50,51,57]. Explicit filtering for LES would also solve this difficulty, but is not in widespread use for reasons of tractability and theoretical development. Level set methods have already been successfully integrated into multi-regime flamelet mapping approaches, but further development work is needed in this area.

4. DIRECTIONS FOR PARTIALLY PREMIXED COMBUSTION MODELING

The discussion in section 3 of how combustion models for LES deal with partially premixed behavior highlights two points. First, it is not yet known how errors in describing partially premixed combustion behavior on the subfilter scale will translate to, and appear in, the statistics of relevant predicted quantities. In some instances, neglecting partially premixed behavior in favor of a simplified modeling approach may provide an adequate engineering analysis. But in many other cases, the predicted flame stability, flame position, scalar variance, and pollutant signature is likely to be considerably affected. The second point is that a variety of tools for answering questions about partially premixed behavior are beginning to appear in the numerical combustion research field. This is encouraging from a modeling perspective, and suggests that dealing with this issue is a tractable problem. In this brief section, a few particular interesting aspects of this process will be considered, and an example of an attempt in LES to account for multiple regimes will be shown.

As discussed in section 2, the task of capturing the thin-flame physics associated with premixed combustion has historically been very difficult for turbulent combustion models. This difficulty arises due to the lack of LES resolution at these scales, and due to the fact that turbulence can disrupt the transport and chemistry balance in the small-scale preheat zone and affect flame speeds in very non-linear ways. In partially premixed combustion, these challenges all remain. But an interesting shift in perspective occurs in this mixed regime. From a certain partially premixed point of view, thin flames are the less challenging, canonical case, and broadened, more homogenized flames are the more difficult case to describe. As partially premixed model development proceeds, it will be interesting to determine whether the resolved scales in an LES will facilitate improved descriptions of these broadened more homogenized flames, or whether these flames will indeed be more challenging to describe than the pure premixed limit. It is likely that the reaction zones in so-called broadened flames cannot be captured with a single regime approach. But conversely, it is not clear that these flames can be accounted for without close attention to the small-scale chemistry and transport interactions that govern combustion physics. As such, it will be important to continue developing improved single regime, and especially improved premixed approaches, for LES. These approaches may inform the most important pieces of new partially premixed models.

Before some brief conclusions are described, a combustor case that highlights an example of a partially premixed model will be briefly discussed. In Fig. (**3**), a flamelet-based LES of NASA's Lean Direct Injection combustor [15] is depicted. Liquid Jet-A fuel is injected into the combustion chamber through an atomizer that sits along the centerline of the swirl assembly. Pure air is injected through the helicoidal swirl vanes of the assembly. The combustor chamber cross section is 2 inches x 2 inches, and the Reynolds number based on the half-width of the chamber and the air injection velocity is Re=31,000. The simulation of this combustor requires modeling the processes of spray injection, spray evaporation, detailed chemistry, radiation, and pollutant formation. Moreover, a case such as this is a particularly challenging test for a partially premixed combustion model. This is because the interaction of the intense shear layer and the pure fuel being evaporated from the spray will produce regimes of both non-premixed and premixed combustion.

The LES of the combustor was performed using a 7.4 million cell mesh, and the simulation was run in parallel on 80 processors for approximately two weeks. While expensive, simulations of this complexity can currently be considered in industrial settings. Large-scale simulations such as this are increasingly affecting the design of industrial turbomachinery products [58].

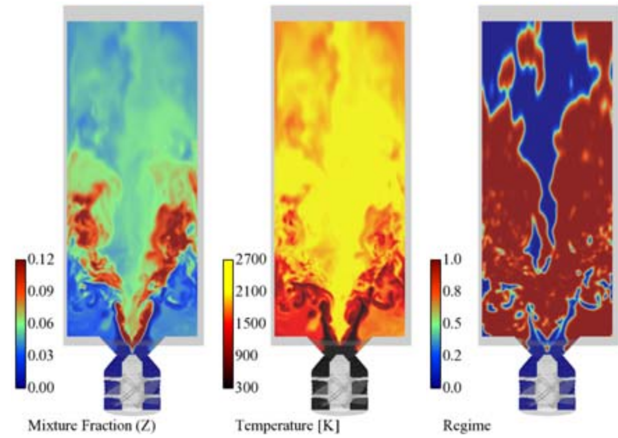

Fig. (3). LES of NASA's LDI spray combustor. Left: Filtered mixture fraction field. Middle: Filtered temperature field. Right: Filtered combustion regime indicator (see section 3.5) with red representing premixed and blue representing non-premixed combustion.

In the simulation, the combustion regime index from section 3.5 is used to map premixed and non-premixed flamelet solutions into the flow. The plot on the right in Fig. (**3**) shows the regimes that are predicted by this index. Both regimes appear to play an important role in determining the combustor's behavior, especially near the swirl assembly and primary reaction zone.

The NASA LDI combustor is laboratory scale and does not rival the complexity of a realistic engine. But realistic aircraft and automotive engines, although more complex, behave according to the same physical processes that are observable in the LDI rig. The opportunity therefore now exists to use data sets such as this to develop fundamentally consistent, predictive combustion models for mixed regimes.

CONCLUSIONS

Partially premixed combustion is highlighted in this article as one of the most relevant and important modeling challenges in the field of turbulent combustion. The partially premixed regime appears in a variety of flame stabilization processes, and therefore in a variety of modern combustion devices. Trustworthy models for this regime will be required to predict and more optimally control the pollutant, noise, efficiency, and stability profiles of future engines.

An analysis of how modern LES combustion models deal with partially premixed behavior has been presented. Because no asymptotically targeted partially premixed models are available, the analysis focused on the advantages and disadvantages that modern approaches have in dealing with mixed regimes. The analysis highlighted some advantages and disadvantages of each approach, and supports the mention of two trends. First, the extent to which the small-scale flame structures in partially premixed regimes influence model predictions is not yet well characterized. This makes it difficult to determine the degree to which these structures need to be incorporated into models before they can be considered trustworthy. Second, a wide variety of approaches to partially premixed modeling are being tested, applied, and improved. Further experience with these approaches should aid in the model development process as each encounters either success or failure, and accordingly helps to inform a robust regime independent approach.

It is interesting to note that this range of approaches for LES appears to be currently bounded by the thickened flame approach at one end of the spectrum, which empirically adjusts how flow and chemistry time-scales interact to promote model robustness. At the other end of the spectrum, the multi-regime flamelet model puts emphasis on capturing the correct small-scale turbulence and chemistry interactions. The flamelet approach, however, uses single regime asymptotic limits to describe all chemistry, and therefore does not have access to a truly realistic partially premixed phase space. While the use of single regime asymptotics is an approximation, it is clear that combustion models should be considering small-scale flame structures in a correct manner. These small-scale structures are very different in the different regimes, and accurate models must therefore either be regime targeted, or capable of accounting for regime-dependent flame structures.

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Received: September 09, 2009 Revised: November 03, 2009 Accepted: November 17, 2009