A Laminar Flamelet Approach to Subgrid-Scale Chemistry in Turbulent Flows

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A method is presented whereby filtered chemical species may be modeled in large eddy simulations (LES) of nonpremixed, turbulent combustion. The model is based on the concept of laminar flamelets, and assumes that a filtered mixture-fraction, as well as its subgrid-scale variance and filtered dissipation rate, are known at each grid cell of an LES. The model makes use of the subgrid-scale or "large-eddy" probability density function of the mixture-fraction, which is assumed to follow a beta-distribution. Also, an assumed functional form for the scalar dissipation rate is employed. The model is evaluated by filtering data from direct numerical simulations (DNS) of homogeneous, isotropic, decaying turbulence. Results show that the model, termed the large-eddy, laminar flamelet model (LELFM), is reasonably accurate and that the accuracy improves with increasing Damköhler number. © 1997 by The Combustion Institute

1. INTRODUCTION
In nonpremixed turbulent combustion, the large eddies set the rate of mixing and, therefore, the overall rate of product formation. The largest mixing-controlling eddies in a turbulent flow contain most of the turbulent kinetic energy and generally depend on the particular flow configuration. The small scales, on the other hand, contain a small portion of the total energy, are more isotropic than the large scales, and are thought to be more universal in nature. Recent advances in computer technology have made it practical to compute the large eddies in a turbulent flow directly, so that only the small (unresolved) scales need be modeled. This is accomplished by prefiltering the governing equations to eliminate the scales of motion smaller than those resolvable on the computational mesh. This produces equations analogous to the Reynolds-averaged equations, only the extra terms now represent the effects of subgrid-scale motions. Models are proposed for the unknown terms, and then the equations are solved for the resolvable scales of motion (large eddies). This technique, known as large eddy simulation (LES) [1, 2] is expected to be more accurate than calculations employing the Reynolds- (ensemble) averaged equations since the large scales are treated directly.

Several methods have been proposed to account for subgrid-scale mixing and chemical reaction in an LES [3]. One such method is the linear eddy model of Kerstein and co-workers [4, 5]. In this approach, all relevant length scales are resolved in one dimension. Molecular diffusion is treated explicitly and turbulent stirring is modeled by a stochastic rearrangement process applied to a scalar field along the linear domain. The subgrid stirring process involves Monte-Carlo simulations at each grid cell of an LES and hence is very computationally intensive. Gao and O'Brien [6] have derived the equation for the large eddy probability density function (LEPDF) of the various chemical species. Although important for theoretical considerations, this equation appears to be difficult to solve in an LES. In fact, one method of solution is a Monte-Carlo scheme, possibly with a Langevin model similar to the method of Kerstein. An alternative and computationally less intensive approach involves assuming a functional form for the LEPDF of a mixture-fraction [7]. For the case of equilibrium chemistry, this method requires that a filtered scalar, as well as its subgrid-scale variance, be computed as part of the LES.

The primary difficulty in applying LES to turbulent flows with finite-rate chemistry is that chemical reactions generally take place below resolved (grid) scales and hence must be modeled in their entirety. Therefore, it is necessary to obtain an accurate physical description of
the unresolved (subgrid-scale) reaction processes. One way to picture the small-scale reaction zones is as an ensemble of laminar flamelets [8]. This paper uses the laminar flamelet concept to extend a previous subgrid-scale model for equilibrium chemistry in an LES [7] to include the case of finite-rate chemistry.

2. LES MODEL

Consider an LES of a nonpremixed chemical reaction in a turbulent flow. In describing the problem, all quantities are nondimensional except those denoted with an asterisk. An overbar denotes a filtered quantity and a prime denotes a small-scale fluctuation, e.g., \( \bar{Z} = \bar{Z} + Z' \). Also, no distinction in notation is made between a random variable and the values that it can take on. Presently, we consider incompressible, isothermal turbulence in which fuel and oxidizer combine, in a single irreversible step, to form product, i.e., Fuel + (r)Oxidizer \( \rightarrow \) (1 + r)Product. Here, \( r \) is the amount of oxidizer that disappears upon reaction with a unit mass of fuel.

Let \( Y_f \) and \( Y_o \) denote mass fractions of fuel and oxidizer, respectively. They satisfy

\[
\frac{\partial Y_f}{\partial t} + \bar{u} \cdot \nabla Y_f = \frac{1}{Pe_f} \nabla^2 Y_f - \dot{w}_f, \tag{1}
\]

\[
\frac{\partial Y_o}{\partial t} + \bar{u} \cdot \nabla Y_o = \frac{1}{Pe_o} \nabla^2 Y_f - \dot{w}_f, \tag{2}
\]

with the reaction rate given by

\[
\dot{w}_f = Da Y_f Y_o. \tag{3}
\]

Here, the Peclet and Damköhler numbers are defined by

\[
Pe_f = \frac{L^* U^*}{D^*_f}, \quad Pe_o = \frac{L^* U^*}{D^*_o},
\]

\[
Da = \frac{K^* L^*}{U^*},
\]

where \( L^* \) is a reference length scale, \( U^* \) is a reference velocity scale, \( D^*_f \) and \( D^*_o \) are the diffusivities of fuel and oxidizer, respectively, and \( K^* \) is a reaction rate constant.

A mixture-fraction \( Z \) can be defined as [9]

\[
Z_f = \frac{Y_o}{r + \frac{Y_o2}{r}} \frac{Y_o}{Y_f + \frac{Y_o2}{r}}, \tag{4}
\]

where \( Y_{f1} \) is the mass fraction of fuel in the fuel stream and \( Y_{o2} \) is the mass fraction of oxidizer in the oxidant stream. From Eqs. 1 and 2, assuming equal diffusivities, i.e., \( D^*_f = D^*_o = D^* \), the mixture-fraction is easily shown to satisfy the advection diffusion equation:

\[
\frac{\partial Z}{\partial t} + \bar{u} \cdot \nabla Z = \frac{1}{Pe} \nabla^2 Z, \quad Pe = \frac{L^* U^*}{D^*}. \tag{5}
\]

We consider a grid-scale volume element in which a chemical reaction is possibly taking place. We assume that the reaction occurs in thin flames that are locally one-dimensional, and that the flow field is locally counterflow. The existence of a thin flame (a laminar flamelet) has been argued by Peters [8], based on Da being large. The thin flame is located in the vicinity of the stoichiometric surface, defined by

\[
Z(x', t) = Z_{st} = \frac{r Y_f^2}{r Y_f^2 + r Y_o^2}. \tag{6}
\]

Due to the dynamics of the scalar gradient vector, there is a strong tendency for the constant \( Z \) surfaces to align orthogonal to the most compressive principal axis of the strain rate field [10]. Furthermore, recent experimental data have indicated that, for high Reynolds numbers and for Peclet numbers of order 1 and larger, the \( Z \)-field consists of very thin regions of large \( X \), separated by regions of more uniform \( Z \) [11]. Here, \( X \) is the scalar dissipation rate, defined by \( X = (1/Pe)\nabla Z \cdot \nabla Z \).

Assuming the flame is locally steady, and that \( Z \) is a monotonic function of the local coordinate normal to the flame, \( Y_f \) can be expressed in terms of \( Z \), and Eqs. 1 and 5 combine to give [8]

\[
\chi(Z, t) \frac{d^2 Y_f}{dZ^2} = \dot{w}_f. \tag{7}
\]
The effects of the local turbulent straining field are contained in \( Z \) and \( \chi \). Several terms have been neglected in Eq. 7, based on the assumption that the reaction is fairly fast and the reaction layers are thin, so that the second derivative and reaction rate terms dominate the equation. According to laminar flamelet theory [8], for large Da only the value of \( \chi \) at the stoichiometric surface, say \( \chi_{st} \), is important, so that Eqs. 7 can be integrated, at least in theory, to give \( Y_f = Y_f(Z, \chi_{st}) \). The oxidant is related to \( Y_f \) and \( Z \) via

\[
Y_o = Y_oZ(1 - Z) + r(Y_f - Y_f1Z). \tag{8}
\]

Analysis of direct numerical simulation (DNS) data [12] and laboratory data [13] indicate that it is important to consider the functional dependence of \( \chi \) near the flame, and that, indeed, this may extend the range of validity in Da of the results. Peters [8] has suggested that \( \chi(Z, t) \) can be modeled by the laminar counterflow, i.e.,

\[
\chi = \chi_0 F(Z), \tag{9}
\]

where \( \chi_0 \) is the local peak of \( \chi \) within the layer, and \( F \) is given by

\[
F(Z) = \exp(-2[\text{erf}^{-1}(2Z - 1)]^2). \tag{10}
\]

Here, \( \text{erf}^{-1} \) is the inverse error function (not the reciprocal). Southerland and Dahm [13] have suggested that Eq. 10 is only valid in those regions of the flow where unmixed fuel and oxidizer are present, i.e., \( Z \) takes on values of 0 and 1. Far downstream in a turbulent flow, all fluid may be at least partially mixed; in this case, \( \chi \) will go to zero at the local minimum and maximum values of \( Z \). Local minimum and maximum values of the scalar field are denoted by \( Z^- \) and \( Z^+ \), which represent values of \( Z \) in locations where \( \nabla Z = 0 \). In an attempt to account for regions where \( Z^- > 0 \) and/or \( Z^+ < 1 \), Southerland and Dahm have introduced a scaled form of Eq. 10 with zeros at \( Z = Z^- \) and \( Z = Z^+ \) rather than at \( Z = 0 \) and \( Z = 1 \). Our findings suggest that Eq. 10 is adequate for the model presented herein. In Section 5, some justification of this assumption will be given based on observations from DNS data.

Using the boundary conditions:

\[
Y_f(Z = 0, \chi_0) = 0, \tag{11}
\]
\[
Y_f(Z = 1, \chi_0) = Y_f1, \tag{12}
\]

Eq. 7 can be solved to obtain \( Y_f(Z, \chi_0) \). If fresh fuel and/or oxidizer are not present within an LES grid cell, the applicability of Eqs. 11 and 12 is not obvious. In a reacting flow, \( Y_f \) should approach the equilibrium limit at \( Z = Z^- > 0 \) and/or \( Z = Z^+ < 1 \) since \( \chi(Z^-) = \chi(Z^+) = 0 \). The equilibrium model for \( Y_f \) also obeys Eqs. 11 and 12, therefore, these boundary conditions are always appropriate. By assuming that reactions occur in thin regions of one-dimensional counterflow, the \( Z \) dependence of \( \chi \) is known (see Eq. 9). Furthermore, by assuming that \( Z^- = 0 \) and \( Z^+ = 1 \), \( \chi_0 \) then represents the value of \( \chi \) where \( Z = 0.5 \). The assumed form for \( \chi \) thus implies that \( \chi_0 \) is independent of \( Z \) and that \( \bar{Y}_f \) can be expressed as

\[
\bar{Y}_f = \int_0^1 \int_{\chi_o}^{\chi_o \text{max}} Y_f(Z, \chi_0) P(\chi_0) P(Z) d\chi_0 dZ, \tag{13}
\]

where \( \chi_o \text{min} \) and \( \chi_o \text{max} \) are the minimum and maximum values of \( \chi_0 \) within the subvolume. Note that the range of \( \chi_0 \) within a subvolume may be much smaller than the range of \( \chi \) within a subvolume.

We next make use of an observation similar to one made by Kuznetsov and Sabel'nikov [14], which is that, within the interval of integration \( \chi_o \text{min} \leq \chi_0 \leq \chi_o \text{max} \), \( Y_f \) is a weak, approximately linear, function of \( \chi_0 \). Therefore, \( Y_f(Z, \chi_0) \) can be approximated by the first two terms in the Taylor series expansion about the average of \( \chi_0 \), i.e.,

\[
Y_f(Z, \chi_0) \approx Y_f(Z, \bar{\chi}_0) + \frac{\partial Y_f}{\partial \chi_0} \bigg|_{\chi_0} (\chi_0 - \bar{\chi}_0). \tag{14}
\]

Inserting Eq. 14 into 13 and integrating over \( \chi_0 \) gives

\[
\bar{Y}_f = \int_0^1 Y_f(Z, \bar{\chi}_0) P(Z) dZ. \tag{15}
\]
Similar relationships can be obtained for \( \bar{Y}_o \) and for \( \bar{Y}_p \), the filtered value of the product mass fraction. Note that \( \bar{X}_o \) is obtained in terms of \( \bar{X}, F(Z), \) and \( P(Z) \) by averaging Eq. 9, i.e.,

\[
\bar{X}_o = \frac{\bar{X}}{\int_0^1 F(Z)P(Z)dZ}.
\]  

(16)

In order to determine \( \bar{Y}_f \), \( P(Z) \) is still needed. The LEPDF, appearing in the integrals in Eqs. 15 and 16, is assumed to follow a beta-distribution \[7\], i.e.,

\[
P(Z) = \frac{Z^{a-1}(1-Z)^{b-1}}{B(a, b)},
\]

where \( B(a, b) \) is the beta function and \( Z^2 \) is the subgrid-scale variance of \( Z \). Note that \( Z^2 \) is not necessarily equal to \( Z^2 \). In filtering DNS fields, in order to simulate LES data, the subgrid-scale variance should be computed as the mean-of-the-square minus the square-of-the-mean, rather than as the mean-square of the fluctuation. The latter approach is incompatible with the beta model for the LEPDF and has been found to cause errors in the results. Furthermore, in the beta-PDF model, \( \bar{Z} \) and \( Z^2 \) represent the first two moments of a random variable; therefore, the filter kernel must be positive definite in physical space \[6, 7\]. For example, a Fourier truncation filter is not appropriate for evaluating the present model, because Gibb's phenomenon may cause \( \bar{Z} \) to lie outside the range \( 0 \leq \bar{Z} \leq 1 \).

3. SUMMARY OF METHODOLOGY

Prior to running an LES, the model is used to construct a table for \( \bar{Y}_f \) based on \( \bar{Z}, Z^2 \), and \( \bar{X} \). It is assumed that \( \bar{Z}, Z^2 \), and \( \bar{X} \) are obtainable at each grid point of a large-eddy simulation. The steps in setting up the table are as follows:

1. Choose values for \( \bar{Z}, Z^2 \), and \( \bar{X} \).
2. Compute \( F(Z) \) from Eq. 10 and \( P(Z) \) from Eq. 17.
3. Use Eq. 16 to solve for \( \bar{X}_o \).
4. Replace \( \chi(Z, t) \) with \( \chi F(Z) \) in Eq. 7 and use the boundary conditions in Eqs. 11 and 12 to solve for \( Y_f(Z, \bar{X}_o) \). This can be accomplished numerically using either a shooting or a relaxation scheme \[15\].
5. Insert \( Y_f(Z, \bar{X}_o) \) and \( P(Z) \) into Eq. 15 and integrate numerically to obtain \( \bar{Y}_f(\bar{Z}, Z^2, \bar{X}) \).
6. Repeat steps 1–4 for the full range of \( \bar{Z}, Z^2 \), and \( \bar{X} \) expected from the LES, in order to construct a table for \( \bar{Y}_f \).

Steps 1–5 represent a fairly lengthy but one-time process. The tabulated values of \( \bar{Y}_f \) will depend on the parameters \( r, Y_{f1}, \) \( Y_{o2}, \) \( P_e \), and \( Da \) of the LES. Once the table is constructed, the model may be applied in an LES by using \( \bar{Z}, Z^2 \), and \( \bar{X} \) at each LES grid point to look up \( \bar{Y}_f \) by tri-interpolation. The mass fractions of the grid-scale oxidizer and product can then be computed as

\[
\bar{Y}_o = Y_{o2}(1 - \bar{Z}) + r(\bar{Y}_f - \bar{Z}Y_{f1}),
\]

\[
\bar{Y}_p = (r + 1)(\bar{Z}Y_{f1} - \bar{Y}_f).
\]

(18)

(19)

4. RESULTS

In order to investigate the accuracy of the model, data sets from high-resolution, direct numerical simulations are used. The DNS fields are filtered to obtain exact values for \( \bar{Y}_p, \bar{Z}, Z^2 \), and \( \bar{X} \) at each point of a hypothetical LES mesh. The latter three quantities are then used to obtain model values for \( \bar{Y}_f \) via trilinear interpolation of the look-up table. For the results presented herein, the DNS mesh consists of \( 128 \times 128 \times 128 \) grid points, and the LES mesh consists of \( 16 \times 16 \times 16 \) grid points. Thus, each point in the LES grid is composed of a box-average of \( 8 \times 8 \times 8 \) DNS grid points.

Results from three sets of data are presented and will be denoted as cases A, B, and C. The data fields were taken from Mell et al.'s temporal simulations of isotropic, decaying tur-
The following table lists the important parameters for each case.

In the table, $\Delta$ represents the filter width, i.e., LES grid spacing. The integral, Taylor, and Kolmogorov microscales of the turbulence [17] are denoted by $l$, $\lambda$, and $\eta$, respectively. Quantities in angle brackets represent averages over the entire flow field. $Sc$ is the global Schmidt number and $Da_t$ and $Re_t$ are the turbulent Damköhler and Reynolds numbers, respectively. The quantity $\langle Z \rangle - \langle Z \rangle^2$ defines the maximum possible value of the total variance $\langle Z^2 \rangle - \langle Z \rangle^2$, so that, in the fifth row of the table, a value of 1 would correspond to completely segregated reactants, and a value of 0 would mean that the reactants are completely mixed. In the definitions for $Sc$, $Da_t$, and $Re_t$, $\nu^*$ is the kinematic viscosity and $u_{rms}^*$ is the root-mean-square of the velocity fluctuations. The rms velocity is computed by averaging over the entire $128 \times 128 \times 128$ point data set. Cases A and B are taken from the same simulation, A at 0.27 large-eddy turnover times, and B at 1.9 large-eddy turnover times. These times were computed by integrating the instantaneous large-eddy turnover time from the start of the simulation, i.e.,

$$t_{le} = \int_0^t \frac{u_{rms}}{l} \, d\tau.$$  \hspace{1cm} (20)

Figure 1 shows the correlation of exact and model values for the fuel, oxidizer, and product for case A, with a Damköhler number of 2.1.

### Table

<table>
<thead>
<tr>
<th>Parameter</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta/l$</td>
<td>0.445</td>
<td>0.366</td>
<td>0.445</td>
</tr>
<tr>
<td>$\Delta/l$</td>
<td>1.33</td>
<td>0.990</td>
<td>1.33</td>
</tr>
<tr>
<td>$\Delta/\eta$</td>
<td>18.5</td>
<td>11.9</td>
<td>18.5</td>
</tr>
<tr>
<td>$\langle Z \rangle$</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>$\langle Z^2 \rangle - \langle Z \rangle^2$</td>
<td>0.824</td>
<td>0.183</td>
<td>0.824</td>
</tr>
<tr>
<td>$Z_{st}$</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>$Sc = \frac{\nu^<em>}{D^</em> \lambda}$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$Da_t = \frac{u_{rms}^<em>}{K^</em> \lambda}$</td>
<td>2.1</td>
<td>4.54</td>
<td>8.4</td>
</tr>
<tr>
<td>$Re_t = \frac{u_{rms}^* l^<em>}{\nu^</em>}$</td>
<td>148</td>
<td>101</td>
<td>148</td>
</tr>
</tbody>
</table>

Each point in the plot corresponds to one LES grid point. The plots on the left show the predictions of the model discussed in Section 2, which is called the large-eddy, laminar flamelet model (LELFM). The plots on the right show the results of assuming frozen (no reaction) and equilibrium (infinite Damköhler number) chemistry. These limits provide a reference for judging the model’s performance. In the frozen limit, the filtered fuel is $Y_f = Y_{f1} Z$, while in the equilibrium limit it is modeled as [7]

$$\frac{Y_f}{Y_{f1}} = \int_{Z_{st}}^1 \frac{(Z - Z_{st})^{b-1}}{B(a, b)} \, dZ,$$

\[= \frac{aI_{1-Z_{st}}(b, a + 1)}{(a + b)(1 - Z_{st})} - \frac{Z_{st}I_{1-Z_{st}}(b, a)}{1 - Z_{st}}. \]  \hspace{1cm} (21)

where $I_{a}(\alpha, \beta)$ is the incomplete beta-function. Since $Z_{st} < 0.5$, the limits for the fuel are closer together than the limits for the oxidizer. Figure 2 shows the model’s performance at a later time in the same simulation, where the Damköhler number has increased by about a factor of 2. The predictions are significantly improved. Figure 3 shows results at the same point in time as case A, but with a Damköhler number of 8.4. Note the improvement of both the LELFM and the equilibrium predictions. The model has also been applied to data from a DNS of a turbulent reactive plume [18] in which $Z_{st} = 0.111$ and $\langle Z \rangle = 0.00607$, with essentially the same results.

### 5. THE DEPENDENCE OF $\chi$ ON $Z$

Bray and Peters [19] note that, in recent applications of laminar flamelet modeling, $\chi$ has been customarily replaced by its average. Both Bray and Peters [19] and Kuznetsov and Sabel’nikov [14] agree that this procedure is misleading. Indeed, using the DNS data, we have found that if $\chi$ is replaced in Eq. 7, either by $\bar{\chi}$ or by $\chi_{st} = \chi_{st}F(Z_{st})$, significant errors result. This is because in reality, $\chi$ is zero in regions of pure fuel or oxidizer. If unmixed fuel and/or oxidizer are present in the subgrid-scale volume, then $P(Z)$ will ap-
Fig. 1. Correlation of exact and model species mass fractions for case A.

Approach a delta function at 0 and/or 1. For these grid cells, the modeled value of \( \chi_0 \) (e.g., see Eq. 16), will be incorrect unless the assumed form for \( \chi \) has the properties \( \chi(Z = 0) = 0 \) and \( \chi(Z = 1) = 0 \).

The success of the counterflow model, as stated in Eq. 10, appears to be related to the fact that it accurately predicts the subgrid-scale conditional average of \( \chi \) for the range of \( Z \) where \( P(Z) \) is large. Using Eqs. 9 and 16, the following model is obtained for the conditional dissipation rate:

\[
\frac{\chi(Z)}{\bar{\chi}} = \frac{F(Z)}{\int_0^1 F(Z) P(Z) dZ}.
\]
The effectiveness of this model is examined in Fig. 4, which compares \( \chi \frac{Z}{\chi} \), computed directly from the DNS data, with \( F(Z)/\int_{0}^{1} F(Z) P(Z) dZ \). Also shown are \( P(Z) \) obtained directly from the data and \( P(Z) \) from the beta-model. The plots on the left-hand side show results from LES grid-scale volumes taken from case A at three different spatial locations. It can be seen that \( Z \) takes on the values of 0 and 1 within the regions, and that \( F(Z) \) and \( P(Z) \) match the DNS data quite well. The plots on the right-hand side show the same sub-volumes later in time (case B). It can be seen that \( Z \) no longer takes on the values of 0 and 1,
meaning that $Z^- > 0$ and $Z^+ < 1$. The plots show that $F(Z)$ is reasonably accurate where $P(Z)$ is large, and that $F(Z)$ overpredicts $\chi |Z$ only where $P(Z)$ is small. Note that LELFM was found to be more accurate for case B than case A, even though $F(Z)$ is seen here to be more accurate for case A than case B.

There are several possible reasons why the chemistry model is least accurate for the early stages of mixing: In case A, there may be some remaining effects of the initialization, since $Y_f$ was initially set to the frozen chemistry value. Also, since $Z$ is initialized as random “blobs” of zeros and ones, the box-averaged scalar
dissipation rate $\langle \chi \rangle$ does not reach its peak until near 1 eddy turnover time. Therefore, the layer-like structure of $Z$ and $Y_f$ may not have had time to fully develop. Another possibility is that the neglected time derivative in Eq. 7 is important during the initial mixing when the turbulence is strongest. Bish and Dahm [20], however, suggest that errors in laminar flamelet theory can be removed at low Da if the probability densities of $Z^-$ and $Z^+$ are taken into account. This seeming contradiction may be due to differences in the flows from which the data are taken. Bish and Dahm examined a small region downstream in a turbulent jet where the unsteady term may be less important, and where the layer-like structure of $Z$

![Graphs showing comparisons of model predictions with data from DNS for $t_\sigma = 0.27$ and $t_\sigma = 1.9$.](image)

**Fig. 4.** Comparison of the counterflow model for $\chi$ and the beta-model for the LEPDF with data from the DNS.
appears to be more prominent than in the DNS.

6. CONCLUSIONS

Using DNS data, we have demonstrated the feasibility of applying LES to nonpremixed, turbulent, reacting flows. This is accomplished by using a model for the filtered chemical species. The subgrid-scale chemistry model is based on laminar flamelet theory, and hence is termed the large-eddy, laminar flamelet model. It is computationally inexpensive, and requires as input, values of the filtered mixture-fraction, as well as its subgrid-scale variance and dissipation rate. The predictions of the model are substantially more accurate than what would be obtained by assuming equilibrium chemistry. The model tends to overpredict the product; however, its accuracy improves with increasing Damköhler number. Finally, it was demonstrated that the counterflow model for $\chi$ is acceptable with zeros chosen at $Z = 0$ and $Z = 1$.

The model presented herein has recently been extended to the case of low Mach number combustion in an open domain [21]. The theory and assumption necessary for treating variable density, turbulent combustion with multistep, temperature-dependent reactions will be reported in a future work [22]. In particular, the effects of Arrhenius kinetics and reaction stoichiometries on the chemistry model are being investigated. The ability of the model to predict filtered reaction rates is also being examined.

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REFERENCES