A Discrete Dynamical System Subgrid-Scale Model for LES of Turbulent Combustion

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Abstract
We present results of preliminary analyses pertaining to a subgrid-scale (SGS) model for reacting flows which can be used in the context of large-eddy simulation (LES). In a non-classical approach to LES (as described herein), SGS solutions are modeled directly, instead of their correlations, by employing discrete dynamical systems (DDSs) derived from governing equations. The present work serves as a continuation of analysis begun by Holloway et al. (in Proc. 2003 Western States Section Combustion Institute Tech. Meeting), with the addition of variable density to the model used in that work. Results are presented in the form of time histories and two-dimensional bifurcation diagrams.

Introduction
In spite of the challenges associated with constructing accurate subgrid-scale (SGS) models, large-eddy simulation (LES) has shown promise in simulating several basic “building block” flows and even some flows for engineering applications. However, LES methods, in general, have yet great room for improvement, particularly in the modeling of chemical kinetics on the sub-grid scales. For this reason it is expected that simulation of turbulent reacting flows will remain one of the preeminent challenges for scientific computing in the next few decades.

Recently Zhang et al. [1] used a two-step, reduced reaction mechanism to model H\textsubscript{2}--O\textsubscript{2} combustion on the sub-grid scales. In that work, a discrete dynamical system (DDS) was used as the fluctuating part of an SGS model in the context of LES, and it was able to produce time histories quite similar (qualitatively) to those observed in experimental measurements of H\textsubscript{2}--O\textsubscript{2} combustion. Further investigations of this kind continued in the work of McDonough and Holloway in [2], and then again through analysis of bifurcation diagrams by Holloway et al. [3]. In all of these investigations, the primary concern was the influence of velocity fluctuations on chemical kinetics on the sub-grid scales. Thus in those works the reverse coupling—that is, the influence of SGS chemical kinetics on SGS velocity fluctuations—was not yet considered.

In the present work we supplement analysis of time histories [1] and bifurcation diagrams [3] to specifically account for this coupling. This is done by augmenting the SGS model used in [1]--[3] with a formulation for variable density, as we shall elucidate.

As explained in [1]--[3], we approach the modeling of turbulent reacting flows within the non-classical, alternative context of LES as first introduced by McDonough et al. [4]. More specifically, the SGS model herein is formulated on the premise that solutions, rather than governing equations, are filtered. Such an approach allows fluctuating dependent variables to be modeled directly, rather than their fluctuation correlations, and this is done by employing DDSs derived from governing equations. SGS models developed in this fashion require no unknown modeling parameters, and thus constitute “closed” models for LES.

In the following we briefly review the alternative approach to LES in which the variable-density SGS model is employed. We then present the model and, in particular, its DDS that is capable of engendering turbulent-like behaviors as are commonly found in reacting flows. Next, we illustrate the approach used in augmenting the model used in [1]--[3] to account for variable density, and discuss the significance of its implementation. Finally, we present results produced by this new model in the form of time histories and bifurcation diagrams, and then compare and

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posed by McDonough and Huang [5]. References [1]–[3], as well as the present investigate the qualifications directly for combustion phenomena as first proposed in [4], solutions are filtered—rather than governing equations—but the usual LES decomposition is retained:

\[ Q_t + \nabla \cdot F(Q) = \nabla \cdot G(Q) + S(Q). \]  

(1)

Since not all flow scales can be resolved efficiently, modeling approaches are often employed to solve (1). In accordance with the modeling approach as first proposed in [4], solutions are filtered—rather than governing equations—but the usual LES decomposition is retained:

\[ Q(x, t) = q(x, t) + q^*(x, t), \quad x \in \mathbb{R}^d, \quad d = 2, 3, \]  

(2)

with \( q(x, t) \) and \( q^*(x, t) \) representing the resolved-scale and sub-grid scale contributions, respectively. We follow the approach used in [2] and [3] and model \( q^*(x, t) \) with

\[ q_i^* = A_i M_i, \quad i = 1, 2, \ldots, N_v, \]  

(3)

where \( N_v \) is the number of dependent variables, \( A_i \) \( s \) are amplitude factors derived from Kolmogorov scalings [2], and the \( M_i \) \( s \) are components of a DDS appropriate for the particular problem investigated. A DDS applicable to two-dimensional reacting flows is presented in the following section as (4).

In this context, for each resolved-scale time step, \( q(x, t) \) is calculated directly via (1) using \( Q(x, t) \) from the previous time step. The resulting \( q(x, t) \) is low-pass filtered to correct for aliasing errors, and is then saved as the resolved-scale solution. Next, this \( q(x, t) \) is high-pass filtered, producing information that is used to construct the \( A_i \) \( s \) in (3) and bifurcation parameters appearing in (4) [2]. With these values set, \( q^*(x, t) \) is calculated with (3) and (4). Finally, \( q^*(x, t) \) is added to the low-pass filtered \( q(x, t) \) as per (2), resulting in the complete solution, \( Q(x, t) \), for the current time step.

### Subgrid-Scale Model

Discrete dynamical systems can be derived from governing equations and used to model SGS solutions directly for combustion phenomena as first proposed by McDonough and Huang [5]. References [1]–[3], [5], as well as the present investigate the qualitative behaviors of an SGS model as it is used to simulate \( \text{H}_2-\text{O}_2 \) combustion. We remark, however, that the model herein may just as well be tailored to model other combustion chemistry, as explained in [5]. For brevity, here we simply present the generalized DDS for reacting flows and cite [1] for its derivation, as well as for its more specific form as it pertains to \( \text{H}_2-\text{O}_2 \) combustion.

\[ a^{(n+1)} = \beta_a a^{(n)} (1 - a^{(n)}) - \gamma_a a^{(n)} b^{(n)}, \]  

(4a)

\[ b^{(n+1)} = \beta_b b^{(n)} (1 - b^{(n)}) - \gamma_b a^{(n)} b^{(n)} + \alpha_T c^{(n)}, \]  

(4b)

\[ c^{(n+1)} = \left( \sum_{i=1}^{N_s} \alpha_{Td} d_i^{(n+1)} - \gamma_{aT} a^{(n+1)} \right) \]  

\[ - \gamma_{bT} b^{(n+1)} c^{(n)} - \sum_{i=1}^{N_s} H_i \dot{\omega}_i \right) / (1 + \beta_T) + c_0, \]  

(4c)

\[ d_i^{(n+1)} = - \left( \beta_{Y_i} a^{(n+1)} + \gamma_{aY} b^{(n+1)} \right) d_i^{(n)} + \dot{\omega}_i + d_{i,0}, \quad i = 1, 2, \ldots, N_s, \]  

(4d)

with

\[ \dot{\omega}_i = \sum_{j=1}^{N_s} \left[ C_{f,ij} \prod_{\ell=1}^{N_s} d_{\ell}^{(n,\ell)} - C_{b,ij} \prod_{\ell=1}^{N_s} d_{\ell}^{(n,\ell)} \right]. \]

These nonlinear, algebraic maps retain many of the chaotic behaviors deeply rooted within the original governing equations. In addition, we find that (4) provides an efficient method for approximating SGS solutions that have shown to produce temporal behaviors and bifurcation regimes consistent with laboratory experimentation and direct numerical simulation [1]–[3].

As explained in [1], derivation of (4) leads to the construction of numerous bifurcation parameters \( (\beta_s, \gamma_s, \alpha_s, \text{etc.} ) \), all of which are related to physical quantities associated with the particular flow investigated. When (4) is employed in a complete LES, these parameters are calculated automatically, “on the fly” by using high-pass filtered results of the resolved-scale solution. We note, however, that because of the nature of the SGS model construction per (3), a priori investigations of the model’s behavior may be performed without implementation in LES. Thus here, as in [1]–[3], bifurcation parameters are set to fixed values manually, and (4) is analyzed independently.

### Variable Density Formulation

Until now, investigations involving SGS models employing (4) have assumed constant density, \( \rho \), throughout the flow field [1]–[3]. In the following we consider a means by which to resolve this shortcoming. But in addition, in doing so we at least
partially account for the coupling of this new chemistry back on the velocity field as it appears through the bifurcation parameters of (4).

As explained in [1], $\beta_u$ and $\beta_v$ are related to Reynolds number via

$$\beta_i = 4 \left( 1 - \frac{\tau |k|^2}{Re_i} \right), \quad i = u, v. \quad (5)$$

Here, $Re_i$ is a grid-cell Reynolds number, typically of the same order of magnitude as the Taylor microscale Reynolds number; the discrete time step, $\tau$, and wavevector, $k$, are also associated with this scale. It follows that a perturbation in $\rho$, say $d\rho$, will perturb $\beta_i$s by some $d\beta_i$, and hence will directly influence the velocity field.

Although relatively simple to implement into the SGS model of (3), time and space varying $\rho$ will allow for modeling of a wide range of reacting flows outside the capabilities of its predecessor. Supplementing (4), we provide an equation of state to calculate $\rho$. For simplicity we assume ideal gas behavior, as such may be justified in many combustion systems. Then

$$\rho = \frac{P}{RT}, \quad (6)$$

where $R$ is the local specific gas constant of the bulk fluid; $P$ and $T$ are local pressure and temperature, respectively, of the combustion gases.

We seek a means by which to calculate $d\beta_i$, due to some $d\rho$. To begin, we differentiate (5) with respect to $Re_i$ and find

$$d\beta_i = \frac{4\tau |k|^2}{Re_i^2} dRe_i, \quad (7)$$

where $dRe_i$ is a function of $\rho$. Next, it can be shown by differentiation of $Re_i$ and algebraic manipulation that

$$d\beta_i = \frac{4\tau |k|^2}{Re_i} \left( \frac{1}{\rho} \right) d\rho. \quad (8)$$

Differentiating (6) and assuming (locally) constant pressure leads to

$$d\rho = -\rho \left[ \left( \frac{\partial \rho}{\partial R} \right) dR + \left( \frac{\partial \rho}{\partial T} \right) dT \right]. \quad (9)$$

Finally, after combining (9) with (8) and then observing from (5) that

$$\frac{4\tau |k|^2}{Re_i} = 4 - \beta_i,$$

we arrive at

$$d\beta_i = (\beta_i - 4) \left[ \left( \frac{1}{R} \right) dR + \left( \frac{1}{T} \right) dT \right]. \quad (10)$$

Having devised a means to calculate $d\beta_i$, we must yet explain the context of its implementation. At each time step, $(n)$, of (4), $\beta_u$ and $\beta_v$ will be perturbed by respective $d\beta_i$s as per (10). Then for each new time step, $(n + 1)$,

$$\beta_i^{(n+1)} = \beta_i + d\beta_i^{(n)}, \quad i = u, v, \quad (11)$$

and we see that $\beta_u$ and $\beta_v$ are non-constant throughout iterations of (4). We must clarify here, however, that $\beta_i$ in (10) and (11) are held fixed throughout iterations of (4), because this would be done during each large-scale time step of a complete model.

To summarize, by supplementing (4) with (6)–(11), we may observe how chemical kinetics can directly influence the velocity field on the sub-grid scales.

**SGS Model Results and Discussion**

In this section we discuss the potential of the newly formulated, variable-$\rho$ SGS model to simulate turbulent reacting flows. To begin, we give in Fig. 1 a color legend that will be useful in classifying bifurcation sequences that appear in the bifurcation diagrams that follow.

As more thoroughly discussed in [3], bifurcation diagrams may be used to investigate the potential bifurcation sequences inherent to DDS SGS models. We give, for example, in Fig. 2(a) a bifurcation diagram of the temperature component of (4) constructed by the constant-$\rho$ SGS model used in [1]–[3]. Fig. 2(a) serves as a representative example of the work in [3] in that it illustrates bifurcations of temperature fluctuations as $\beta_u$ and $\beta_v$ are perturbed. Because of the sensitivity to initial conditions inherent to the original governing equations, we would expect implementation of variable $\rho$ to have some affect on the bifurcation regime depicted in Fig. 2(a).

We find, however, in Fig. 2(b), in which the experiment of Fig. 2(a) is repeated with the variable-$\rho$
model, that these affects, at least as modeled herein, are rather miniscule. In comparing Fig. 2(a) with Fig. 2(b), we see essentially analogous bifurcation sequences as $\beta_u$ and $\beta_v$ vary over the range $[2.4:4.0]$, with a few deviations associated with phase-lock behavior appearing in the upper left and central portions of the figures. This can be explained by noting that, while $\beta_u$ and $\beta_v$ are being perturbed by variable-$\rho$, these perturbations are orders of magnitude smaller than the $\beta$s themselves, as will be more clear below.

Having implemented the variable-$\rho$ SGS model, we find turbulent-like fluctuations in the time histories of dependent variables similar to those reported from investigations of experimental measurements and direct numerical simulation. We must be careful, however, to regard these time histories in the sense that they represent SGS model results and not complete solutions. Hence in comparisons to time histories in the literature, they should be viewed as high-pass filtered results of those data; we note, however, by scale similarity that one may still expect the qualitative, structural features to remain similar at both of these scales.

In Fig. 3 we show time history data for $u$ and $v$ velocity components, $\rho$, and $\beta_u$, respectively; these are produced by iterating (4), supplemented with (10) and (11). In this window of the data set, we immediately observe the similarity in the structure of the fluctuations from one component of DDS1 to the next. This is to be expected in the present case, since $\rho$ fluctuations are at most only 2 percent of the mean; also, we observe that the affect of this on $\beta_u$ is even smaller. Nevertheless, this is sufficient to shift both the level and range of the velocity fluctuations, as is readily seen via comparisons with Fig. 4 that displays results produced by the constant-$\rho$ SGS model. We also see a slightly stronger $u$-$v$ correlation in the variable $\rho$ case. At the same time, it is important to recognize that changes in $\rho$ may turn out to be less significant than changes in viscosity due to temperature fluctuations, but this has not been considered here.

Finally, we can deduce from comparing Figs. 5(a)–
(d) with corresponding Figs. 6 that affects of variable $\rho$ have been rather minimal on species concentrations, but we emphasize that these affects have not been introduced into the species’ Peclet numbers because our interest in the present study was direct affect of chemistry on velocity fluctuations. Thus, in comparing Fig. 5 with analogous results reported in [1], one can observe slightly less intermittency; otherwise, results are quite similar.

Summary and Conclusions

In summary, we have presented a LES SGS model that can at least partially mimmick the affects of SGS chemistry back on the SGS velocity field. This was done by supplementing the DDS SGS model used in [1]–[3] with an algorithm that perturbs the DDS’s bifurcation parameters “on the fly” by using information derived from time and space-varying density. The alternative approach to LES as proposed by McDonough et al. [4] was outlined, and a generalized DDS for modeling reacting flows was given for use in this context. Next, a formalism for implementing variable density into this model was explained and discussed before finally presenting results of the new SGS model in the form of time histories and bifurcation diagrams.

We conclude that the variable density formalism presented herein was successful in that it was able to produce noticeable changes in time history fluctuations and bifurcation regimes with respect to the SGS model used in [1]–[3], and these changes in model behavior were not physically unrealistic. We suspect, however, that since variable density did not produce quantitatively significant changes in the behavior of the SGS model, variable transport properties resulting from chemical kinetics may influence the velocity field more so than variable density as
displayed here. Hence in future work it would be beneficial to take these variable transport properties into consideration when constructing SGS models.

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References


