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Regularized deconvolution method for turbulent combustion modeling

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ABSTRACT

The modeling of filtered chemical source terms in large-eddy simulation (LES) of turbulent reacting flows remains a challenge. Deconvolution methods are an attractive technique for representing these unclosed terms. With this technique, filtered scalars are reconstructed through deconvolution. The chemical source terms that are computed directly from the deconvolved scalars are filtered explicitly to represent the turbulence-chemistry interaction. However, the approximate deconvolution method (ADM), frequently employed for non-reacting flows, exhibits shortcomings for reacting scalars. This is because ADM does not ensure essential conservation and boundedness conditions. To address this issue, we propose a regularized deconvolution method (RDM) based on an optimization procedure. We conduct *a priori* and *a posteriori* analyses to examine RDM as a closure in LES. These investigations are performed in the context of explicit filtering. By showing that RDM is accurate and stable with respect to both the filter width and time, we conclude that the new deconvolution method shows promise in application to combustion LES.

1. Introduction

Large-eddy simulation (LES) is now recognized as a viable method for predicting turbulent reacting flows [1]. In most problems involving turbulent reacting flows, the underlying physics is characterized by the dynamics of large-scale flow structures and their interactions with the flame. In LES, large-scale structures are represented explicitly on the computational mesh. By modeling the subgrid scale (SGS) residual contributions, this approach improves descriptions of scalar mixing and turbulent chemistry interaction.

The evolution of reactive flows is described by the solution of the reactive Navier–Stokes equations. Defining $\phi(\boldsymbol{x}, t)$ as a generic reactive scalar, the corresponding transport equation is written as

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x_i}(\rho u_i \phi) = \frac{\partial}{\partial x_i}\left(\rho D_\phi \frac{\partial \phi}{\partial x_i}\right) + \rho\dot{\omega}_\phi, \tag{1}$$

where t is the time, x_i is the spacial coordinate along the ith direction, ρ is the density, u_i is the ith velocity component, D_ϕ is the molecular diffusivity of scalar ϕ and $\dot{\omega}_\phi$ is the source term of ϕ due to chemical reaction. Solving Eq. (1) provides information about ϕ at all scales. To achieve this, the minimum resolution requirement is constrained by the smallest characteristic length scale in the flow field. For instance, the length scale can be determined by the minimum among the Kolmogorov scale, Bachelor scale and the flame thickness, depending on the flow configuration. In LES, the mesh size is characterized by the length scale where the inertial range is resolved [2] instead of resolving the smallest physical length scale. In this approach, reactive scalars need to be filtered by a low-pass filter. Denoting $G(\boldsymbol{x})$ as the time-invariant filter kernel in physical space, satisfying the property $\int_{-\infty}^{\infty} G(\boldsymbol{x})d\boldsymbol{x} = 1$, the explicit filtering of $\phi(\boldsymbol{x}, t)$ is given by the following convolution operation:

$$\overline{\phi}(\boldsymbol{x}, t) = \int_{-\infty}^{\infty} G(\boldsymbol{x} - \boldsymbol{x}')\phi(\boldsymbol{x}', t)d\boldsymbol{x}' =: G * \phi. \tag{2}$$

Hence, the governing equation for a reactive scalar in LES is obtained by applying the low-pass filter G to Eq. (1),

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{\phi}\right) + \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u}_i\widetilde{\phi}\right) = \overline{\frac{\partial}{\partial x_i}\left(\rho D \frac{\partial \phi}{\partial x_i}\right)} + \sigma_\phi + \overline{\rho}\widetilde{\dot{\omega}}_\phi, \tag{3}$$

where $\widetilde{\phi}$ is the Favre filtered scalar, which is defined as

$$\widetilde{\phi}(\boldsymbol{x}, t) = \frac{\overline{\rho\phi}}{\overline{\rho}} =: \widetilde{G} * \phi. \tag{4}$$

Terms on the right-hand-side of Eq. (3) are unclosed; therefore modeling of these terms is required to solve the Favre-filtered LES equation for ϕ. In this paper, we propose closure models for these unclosed terms using the deconvolution method. This approach addresses some of the issues we have in closing these terms, particularly for the filtered chemical source term. The issues are discussed below in this section.

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The filtered molecular diffusion term appearing as the first term on the right-hand-side of Eq. (3) is commonly modeled by retaining first-order terms and neglecting higher order contributions. In general, the closure of this term does not require application of a deconvolution method and takes the following form:

$$\overline{\frac{\partial}{\partial x_i}\left(\rho D_\phi \frac{\partial \phi}{\partial x_i}\right)} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{D}_\phi \frac{\partial \widetilde{\phi}}{\partial x_i}\right). \tag{5}$$

The second term we need to address is the turbulent scalar mixing term, σ_ϕ, which is defined as

$$\sigma_\phi = \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i}\widetilde{\phi}\right) - \overline{\frac{\partial}{\partial x_i}(\rho u_i \phi)}. \tag{6}$$

A typical closure for this term is to use a gradient model [3], which introduces a turbulent diffusivity. A dynamic procedure for evaluating this term has been developed [4].

Modeling of the filtered chemical source term, appearing as last term on the right-hand-side of Eq. (3), is especially challenging. The difficulty arises for two reasons, namely the modeling of chemical reactions and the modeling of the turbulence-chemistry interaction on unfiltered scales. The chemical reactions are usually represented either using detailed or reduced chemistry in Arrhenius form, or relying on reaction-transport manifolds. Examples of combustion models that utilize Arrhenius laws are the artificially thickened flame model [5] and the linear-eddy model [6]. Some examples for manifold-based models are intrinsic low dimensional manifold (ILDM) [7], flame prolongation in ILDM [8], flamelet generated manifold [9], and flamelet progress variable [10]. An adaptive modeling approach that integrates different combustion submodels was developed by introducing a Pareto efficiency [11,12]. In these models, the thermochemical state is represented in terms of a reduced set of scalars. While these methods are effective in reducing the computational complexity of the simulation, they rely on intrinsic assumptions about the underlying flame-structure representation and closure models for the turbulence-chemistry interaction.

To consider effects of turbulence on the combustion process, a closure model is required. For Arrhenius chemistry, models are developed based on large-scale structures. An example for this type of model is the laminar chemistry method [13] which uses the resolved scalars to compute the reaction source term. Other examples are the partially stirred reactor (PaSR) model [14,15] and the scale-similarity closure [16], which extends the laminar chemistry method by modeling the effects of fine-scale structures. In contrast, reaction-transport manifold models typically consider the asymptotic regimes of premixed and diffusion flames. Topology-dependent closures were developed for these models, such as the filtered tabulated chemistry model for LES [17] and presumed probability density function (PDF) models [18]. Although these models have been shown to provide reliable predictions of canonical and complex flame configurations, the dependence on an underlying flame topology limits their application to combustion problems involving a single-flame regime. Therefore, for multi-regime and mixed-mode combustion, submodel adaptation [11,12] or the use of topology-free combustion models is required.

To address this need, turbulent closures using deconvolution methods are considered. Deconvolution methods that are developed from mathematical arguments provide approximate inverse to the filter operation in LES. Consequently, SGS terms in the LES equations can be computed explicitly using the deconvolved variables. Since no assumptions on the reconstructed flow field are made in deriving the deconvolution operator, this approach has the potential to be independent of an underlying flame topology and therefore applicable as subgrid model for both finite rate chemistry and reduced manifold models.

The deconvolution method was first introduced as a closure for the SGS stress terms in LES of non-reactive flows [19], and the method was applied to different flow configurations [20–22]. The application of the deconvolution method to reactive LES was later formulated using a moment-based reconstruction of the scalar field [23–25]. An approximate deconvolution operator derived from a Taylor-series expansion to the Gaussian filter was developed [26]. In conjunction with a flamelet model, this model was applied to a turbulent Bunsen flame.

However, by recognizing that deconvolution operators developed for LES are linear operators, they lack essential boundedness and conservation properties of scalar quantities, which are critical for turbulent reacting flows. By addressing this issue, the objective of this work is to propose a general closure for unclosed terms in Eq. (3) by developing a regularized deconvolution method (RDM). To this end, constraints are directly introduced in RDM to fulfill essential regularization conditions.

The remainder of this paper has the following structure. The governing equations are introduced in Section 2. Section 3 is concerned with reviewing mathematical formulations of classical deconvolution techniques and developing the regularized deconvolution method. We examine the deconvolution methods by considering DNS of a partially-premixed flame in canonically decaying turbulence. The computational configuration is described in Section 4. We first conduct an *a priori* study to quantify the accuracy of the deconvolution methods in terms of scalar reconstruction and the estimation of unclosed terms in Section 5. Then in Section 6 we analyze the performance of RDM in an *a posteriori* study. The paper concludes with an overall evaluation of RDM and its applications in LES in Section 7.

2. Governing equations of LES

In combustion LES, the generic scalar transport equation, shown in Eq. (3), has to be adapted for the temperature and species mass fractions $Y_k, k = 1, \ldots, N_s$, with N_s denoting the number of species. The full set of filtered equations for reactive flows in the low-Mach number limit takes the following form:

$$\frac{\partial}{\partial t}\bar{\rho} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u_i}) = 0, \tag{7a}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{u_j}\right) + \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u_i}\widetilde{u_j}\right) = -\frac{\partial \overline{p}}{\partial x_j} + \frac{\partial \overline{\tau_{ij}}}{\partial x_i} + \sigma_{u_j}, \tag{7b}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{Y_k}\right) + \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i}\widetilde{Y_k}\right) = \overline{\frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)} + \sigma_{Y_k} + \overline{\rho\dot{\omega}_{Y_k}}, \tag{7c}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{T}\right) + \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i}\widetilde{T}\right) = \overline{\frac{1}{C_p}\frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right)} + \sigma_T + \overline{\left(\frac{\rho\dot{\omega}'_T}{C_p}\right)} + \overline{\left(\rho \sum_{k=1}^{N_s} \frac{C_{p,k}}{C_p} D_k \frac{\partial Y_k}{\partial x_i}\right)\frac{\partial T}{\partial x_i}} + \overline{\frac{1}{C_p}\frac{\partial p_0}{\partial t}}, \tag{7d}$$

where p is the hydrodynamic pressure, $C_p = \sum_{k=1}^{N_s} C_{p,k} Y_k$ is the heat capacity of the gas mixture, and $\tau_{ij} = \mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i - 2/3\delta_{ij}\partial u_k/\partial x_k)$ is the viscous stress tensor. Note that Eq. (7 d) is written for low Mach number flow conditions, in which viscous-dissipative effects are ignored, and the thermodynamic pressure p_0 is only a function of time [27], which is evaluated from the state equation.

In this set of equations, Eqs. (7), the divergence of the Reynolds stress tensor σ_{u_j} and the turbulent mixing terms σ_ϕ for $\phi \in \{\boldsymbol{Y}, T\}$ are defined as