Multi-Resolution Analysis of Partially-Stirred Reactor Models for Subgrid Turbulence / Chemistry Interactions.

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Abstract: This paper explores the use of a new technique, termed Multi-Resolution Analysis through Mesh-Sequenced Realizations (MRA-MSR) to examine key model assumptions inherent within partially-stirred reactor (PaSR) subgrid models for finite-rate turbulence / chemistry interactions. MRA-MSR evolves large-eddy simulations on a set of successively-coarsened meshes – the finest mesh provides both a 'truth model' for subsequent analysis and a velocity field which, after filtering, serves to constrain the eddy structures evolved on the coarser mesh levels. Multiple realizations may be performed on each coarse mesh level, allowing an 'on-the-fly' assessment of the effects of subgrid models implemented at these levels. In this abstract, we use multi-resolution data generated from a prior MRA-MSR study of one of the Sydney bluff-body stabilized flames to examine the ability of a PaSR-type closure to model the filtered chemical production rates. Optimization techniques for improving the model response are also explored, and directions for completing the paper are outlined.

Keywords: Subgrid Modeling, Turbulent Combustion.

1 Introduction

The quest for an economical, accurate method to model the effects of unresolved turbulent fluctuations on finite rates of chemical production is a pacing issue in large-eddy simulation of turbulent combustion. Several groups [1] have successfully utilized partially-stirred reactor (PaSR) concepts to model subgrid effects. In such models, the sub-cell environment is divided into fine-scale structures, in which reactions take place, and the remainder, which is assumed to be much less reactive. Interchanges of mass and energy between these environments can be quantified by a general transport equation

$$\bar{\rho}\frac{DY_s^*}{Dt} + \bar{\rho}\frac{(Y_s^* - \tilde{Y}_s)}{\gamma^*(1-\gamma^*)\tau} = \dot{\omega}_s(\bar{\rho}, Y_s^*, \tilde{h}) \tag{1}$$

which is solved for the composition of the fine-scale structures Y_s^*, given filtered-mean density, mass-fraction, and enthalpy information. The closure for the filtered production rates is usually expressed as $\overline{\dot{\omega}_s} = \gamma^* \dot{\omega}_s(\bar{\rho}, Y_s^*, \tilde{h})$. In this work, we focus on an algebraic simplification of (1), given by

$$\bar{\rho}\frac{(Y_s^* - \tilde{Y}_s)}{\gamma^*(1-\gamma^*)\tau} = \dot{\omega}_s(\bar{\rho}, Y_s^*, \tilde{h}) \tag{2}$$

which represents a balance between an interchange-with-the-mean term and the reaction term. As the effective time scale $\gamma^*(1-\gamma^*)\tau$ becomes small, $Y_s^* \to \tilde{Y}_s$ and the closure approaches the 'laminar chemistry' model in which subgrid-scale information is neglected completely. As this time scale becomes large, the reaction source term is driven to zero, and the composition that results is the adiabatic equilibrium solution. For reasons to be outlined in the final paper, the algebraic simplification of the PaSR model has some inconsistencies, and it is perhaps best to dispense with the notion of fine- and coarse-scale structures and instead, regard it as a potential means of determining an alternative average

state that could be used as a replacement for the 'laminar chemistry' model ($\overline{\dot{\omega}_s} = \dot{\omega}_s(\bar{\rho}, Y_s^*, \tilde{h})$ instead of $\overline{\dot{\omega}_s} = \dot{\omega}_s(\bar{\rho}, \tilde{Y}_s, \tilde{h})$). The question is whether this formulation actually captures subgrid effects better.

2 Problem Statement

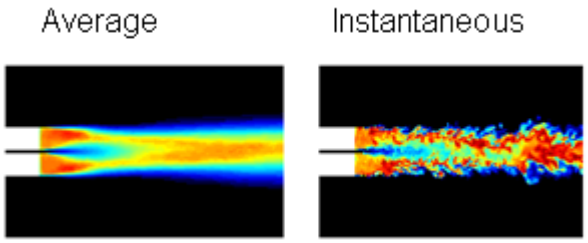

Figure 1: Fine-mesh average and instantaneous temperature distributions for a bluff body stabilized flame

To answer this question, we will employ databases generated using the MRA-MSR procedure [2]. In this method, simultaneous large-eddy simulations are performed on a hierarchy of mesh levels. The velocity field on coarser mesh levels is constrained using a relaxation-type source term dependent on the filtered data from the finest mesh – this allows the eddy structures on all mesh levels to be correlated in space and time. MRA-MSR databases have been obtained for one of the Sydney bluff-body stabilized flames (see Figure 1) – we will use this data to examine several proposed choices for the effective time scale A few results are as follows. We have, from the finest mesh, values for $\bar{\rho}, \tilde{Y}_s, \tilde{h}$, and $\overline{\dot{\omega}_s}$. The first three are used to drive the solution of Eq. (1) at a coarser scale. Time-scale and fine-scale volume-fraction models from the eddy dissipation (ED) variant of PaSR

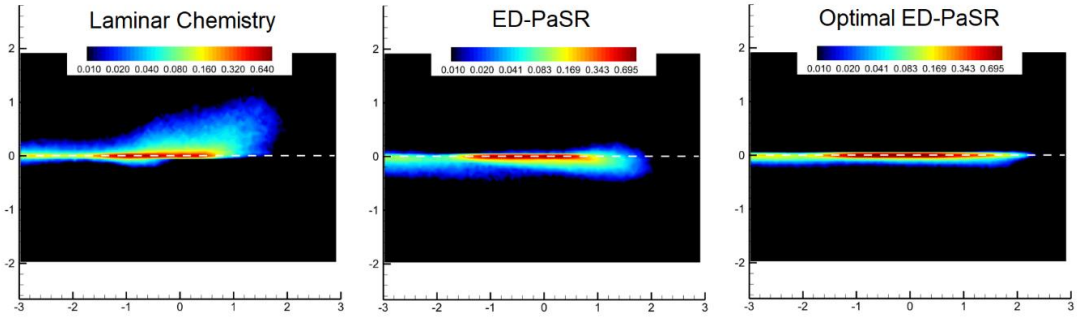

Figure 2: Joint PDF of logarithms of the source term ratio (ordinate) and filtered source term (abscissa)

($\gamma^* = (\mathrm{Re}_\Delta)^{-3/4}$), $\tau = \Delta / (u' \mathrm{Re}_\Delta^{1/2})$ are used. The joint PDF of the ratio $\| \overline{\dot{\omega}_{\mathrm{mod}}} \| / \| \bar{\dot{\omega}} \|$ and $\| \bar{\dot{\omega}} \|$ is plotted in Figure 2 for the laminar chemistry model, the PaSR model, and an 'optimal' PaSR model formulated by introducing a local model constant on the left-hand side of Eq. 2 and finding the value of this constant that minimizes the functional $\sum_s (\overline{\dot{\omega}_{s,\mathrm{mod}}} - \bar{\dot{\omega}}_s)^2$. The ideal solution would be a collapse in the ratio about zero, which is nearly met by the optimal scheme. The original ED-PaSR performs much better than laminar chemistry but tends to under-predict the actual production rate at higher Damköhler numbers.

3 Conclusion and Future Work

The final paper will explore other PaSR variants and will seek to model the 'optimal' response using information extractable from the simulation. Large-eddy simulations of the Sydney flame using the potentially improved PaSR models will conclude the paper.

References

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