A priori Evaluation of Mixing and Reaction Models for LES of Combustion

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This work focuses on validation of Large Eddy Simulation (LES) submodels for scalar mixing and reaction using Direct Numerical Simulation (DNS). Previous attempts at validation of LES combustion submodels using DNS have been limited to simple kinetics (often single-step) and transport. The present study considers DNS of CO/H_2-Air and CH_4/H_2-Air jets using detailed chemical kinetics and mixture-averaged transport. The DNS code used for this study uses 8$^{\text{th}}$ order spatial discretization and a 4$^{\text{th}}$ order Runge-Kutta integrator. *A priori* tests are performed for several LES mixing and reaction models. Beta and clipped-gaussian presumed PDF models are used in conjunction with equilibrium and steady flamelet reaction models to obtain LES state variables such as temperature and species mass fractions. Comparisons are made between filter-scale state variables predicted by the models and the filtered DNS values. The effects of filter size and differential diffusion on model performance are investigated.

In the most abstract sense, reaction models map the state of the system, ϕ_i onto a small set of reaction variables, η_j, $\phi_i = \phi_i(\eta_j)$. The reaction models considered in this study are the equilibrium model (EQ) and steady laminar flamelet model (SLFM). These are coupled with β and clipped-gaussian presumed-shape PDF mixing models, which are parameterized by the mean and variance of the reaction variables. The filtered state variables are then given by

$$\tilde{\phi}_i = \int_{\eta_n} \cdots \int_{\eta_1} \phi_i(\boldsymbol{\eta})\, \widetilde{P}(\eta_1) \cdots \widetilde{P}(\eta_n)\, \mathrm{d}\eta_1 \cdots \mathrm{d}\eta_n. \qquad \textbf{(1)}$$

The tildes in equation 1 indicate Favre-filtered quantities. The EQ model is parameterized by the mixture fraction, $\boldsymbol{\eta} = f$, while SLFM introduces the dissipation rate as an additional reaction variable, $\eta = (f, \chi)$.

These models are tested by first selecting a filter width (Δ) relative to the DNS grid spacing and extracting the Favre-filtered reaction variables (and their variances). Next, the model-predicted state is computed from equation 1, and then compared to the DNS-filtered state variables. When Δ=1 (the DNS scale), the PDF's in equation 1 reduce to δ-functions, and the reaction model alone is the only source of modeling error. As Δ increases, the mixing model begins contributing to the modeling error. Thus, by examining the modeling error as a function of Δ, we may determine the relative error contribution from the mixing and reaction models independently. This is important since in some regions of the flow, the scalar fields may be well-resolved (i.e. the variance of the reaction variables is low and the PDF becomes a δ-function). The modeling error is quantified as the ensemble average of the percent error conditioned on the mixture fraction,

$$\varepsilon = \left\langle \left. \frac{\tilde{\phi}_{\mathrm{DNS}} - \tilde{\phi}}{\tilde{\phi}_{\mathrm{DNS}}} \right|_f \right\rangle. \qquad \textbf{(2)}$$

Standard deviations of this quantity are also considered.

Filter widths up to Δ=16 are considered in evaluating the model performance. For these filter widths, the reaction models are the primary source of error for most state variables. In all cases, SLFM performs better than EQ in prediction of all state variables. Significant shortcomings in SLFM are observed, however, even in cases far from extinction. Shortcomings are attributed to differential diffusion and transient/time-

history effects, neither of which is treated by SLFM or EQ. The attached figures show a brief summary of model performance for temperature for two cases: a CO/H_2 jet and a CH_4/H_2 jet. Figures 1 and 2 show the EQ and SLFM model performance at Δ=1 for the CO/H_2 jet.

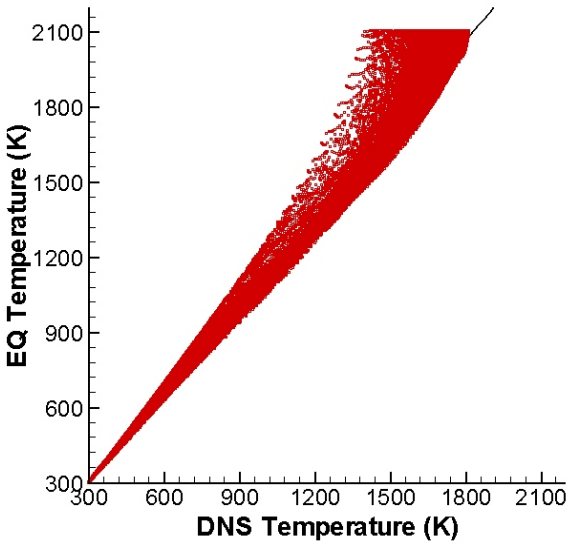

Figure 1 - EQ model performance for CO/H_2 jet.

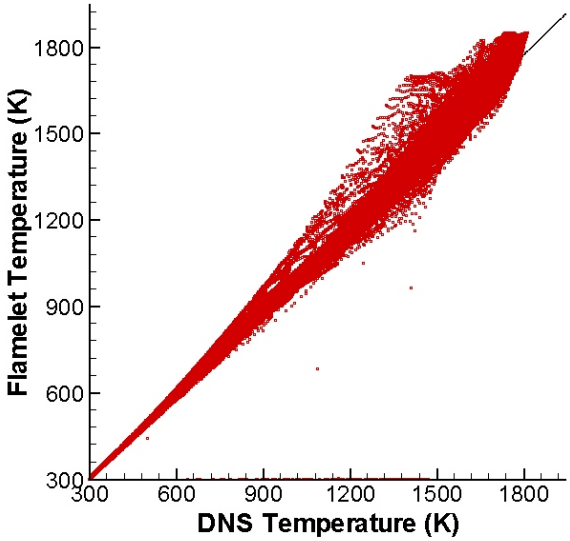

Figure 2 - SLFM model performance for CO/H_2 jet.

Figure 3 shows temperature for the CH_4/H_2 jet. Figure 4 shows conditional percent error as defined by equation 2 for the CH_4/H_2 jet. Interestingly, the largest error occurs away from the stoichiometric mixture fraction. Further analysis shows that this is likely due to differential diffusion.

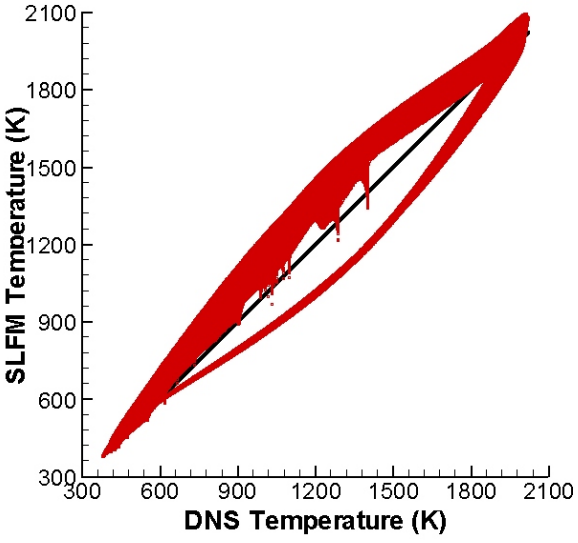

Figure 3 - SLFM performance for CH_4/H_2 jet.

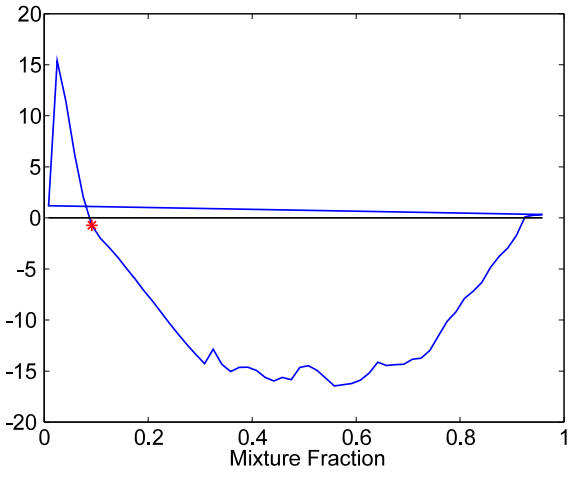

Figure 4 - Conditional percent error on temperature for CH_4/H_2 jet. Red point indicates stoichiometric.