AN EXPLICIT ALGEBRAIC SUBGRID-SCALE SCALAR VARIANCE MODEL

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Abstract We present a subgrid-scale (SGS) scalar variance model based on the explicit algebraic subgrid scalar flux model, EASSFM (8). The EASSFM is a dynamic mixed nonlinear tensor eddy diffusivity model, which is derived from the modeled transport equation of the SGS scalar flux. The explicit algebraic form is obtained using the weak equilibrium assumption. The resulting model improves the direction of the predicted SGS flux vector and enables the prediction of shear-induced SGS fluxes, in contrast with the eddy diffusivity model. The EASSFM has been used for large eddy simulation (LES) of turbulent channel flow with and without system rotation (8; 9) and has been found to improve LES predictions over the dynamic eddy diffusivity model. *A priori* analysis of the EASSFM using the filtered DNS data from a reacting turbulent wall-jet has been performed recently (6; 7), which also showed favorable results. In this study, we evaluate our SGS scalar variance model using the filtered DNS database of a turbulent reacting wall-jet, which is an extension of our previous study on reactive turbulent wall-jet flows (5; 7) to a larger simulation domain. The results show a good agreement between the filtered DNS and our model predictions for the passive and active scalars. This indicates that acceptable predictions of the SGS scalar variance can be obtained using the EASSFM with the new SGS scalar variance model.

FORMULATION OF THE MODEL

The EASSFM for the SGS scalar flux, q_i, of a scalar field, $\widetilde{\theta}$, is expressed as (8; 9)

$$q_i = -(1 - c_{4\theta})\tau^* A_{ij}^{-1} \tau_{jk} \frac{\partial \widetilde{\theta}}{\partial x_k}.$$

In this formulation, $c_{4\theta}$ is a model coefficient, which is computed dynamically, $\widetilde{\cdot}$ denotes a grid-filtered quantity, τ_{jk} is the SGS stress tensor, τ^* is a modeled SGS time scale and the matrix A_{ij}^{-1} is (bold face denotes tensor notation)

$$\mathbf{A}^{-1} = \frac{(c_{1\theta}^2 - \frac{1}{2}Q_1)\mathbf{I} - c_{1\theta}(c_S\widetilde{\mathbf{S}}^* + c_\Omega\widetilde{\mathbf{\Omega}}^*) + (c_S\widetilde{\mathbf{S}}^* + c_\Omega\widetilde{\mathbf{\Omega}}^*)^2}{c_{1\theta}(c_{1\theta}^2 - \frac{1}{2}Q_1) + \frac{1}{2}Q_2},$$

$$Q_1 = c_S^2 tr(\widetilde{\mathbf{S}}^{*2}) + c_\Omega^2 tr(\widetilde{\mathbf{\Omega}}^{*2}), \quad Q_2 = \frac{2}{3}c_S^3 tr(\widetilde{\mathbf{S}}^{*3}) + 2c_S c_\Omega^2 tr(\widetilde{\mathbf{S}}^*\widetilde{\mathbf{\Omega}}^{*2}),$$

where $\mathbf{I}$ is the identity matrix, c_s and c_Ω are model coefficients and $\widetilde{S}_{ij}^*$ and $\widetilde{\Omega}_{ij}^*$ are normalized strain- and rotation-rate tensors. As is customary in RANS (10), for the Reynolds averaged quantities, and in LES (1; 3), for the SGS field, we assume that the ratio of the SGS scalar variance and the SGS scalar dissipation rate is proportional to the SGS time scale $Z_\theta/\varepsilon_\theta = r\tau^*$. The proportionality coefficient that best suits the analysis is $r = 0.45$, which is smaller than the value 0.71 suggested in (1). This difference is due to the difference in the SGS time scale formulation in (1) and the present formulation . If we assume a local equilibrium between the production, dissipation and the source term in the SGS scalar variance equation (3), i.e. $\varepsilon_\theta = -q_i(\partial\widetilde{\theta}/\partial x_i) + \widetilde{\dot{\omega}\theta} - \widetilde{\dot{\omega}}\widetilde{\theta}$ where $\dot{\omega}$ is the reaction rate, we arrive at the following formula for the SGS scalar variance

$$Z_\theta = -r\,\tau^* q_i \frac{\partial \widetilde{\theta}}{\partial x_i} + r\tau^*(\widetilde{\dot{\omega}\theta} - \widetilde{\dot{\omega}}\widetilde{\theta}),$$

where we use the EASSFM for the SGS scalar fluxes. We also use the same modeling for τ^* as is proposed in the EASSFM, which uses a dynamic determination of the SGS kinetic energy and a model for the SGS dissipation.

A PRIORI ASSESSMENT OF THE MODEL USING THE FILTERED DNS DATA

To evaluate the performance of the model, DNS data of a reacting turbulent wall-jet flow is used. The computational domain of the DNS is a rectangular box of size $[L_x \times L_y \times L_z = 48h \times 23h \times 9.6h]$ where L_x, L_y and L_z denote dimensions in the streamwise, wall-normal and spanwise directions, respectively, and h is the inlet jet height, see figure 1. The number of grid points are $[N_x \times N_y \times N_z = 480 \times 288 \times 192]$ and the inlet based Reynolds and Mach numbers of the wall-jet are $Re = 2000$ and $M = 0.5$. At the inlet, fuel and oxidizer enter the domain separately in a non-premixed manner, fuel is injected through the jet, $\theta_{f,j} = 1$, while the oxidizer is injected in the coflow, $\theta_{o,c} = 0.5$. The mean, RMS and the wall-normal scalar flux of the passive scalar, the fuel and the oxidizer species from the DNS are shown in figures 2(a-c) at the downstream position $x = 37\,h$. The DNS data are then filtered using a differential Gaussian filter similar to the approach in (2). The grid and test filter sizes are four and eight times larger than the DNS grid size, respectively.

The new model predictions are compared to those of the dynamic model of (4) (DM) and the filtered DNS data. The mean modeled and exact variance of the scalars at $x = 37\,h$ are shown in figures 3(a-c) where an acceptable agreement between the model predictions and the filtered DNS data is observed.

The new model will be further evaluated using the DNS data and more statistics related to the scalar variance (e.g. probability density function of the prediction error, etc.) will be presented.

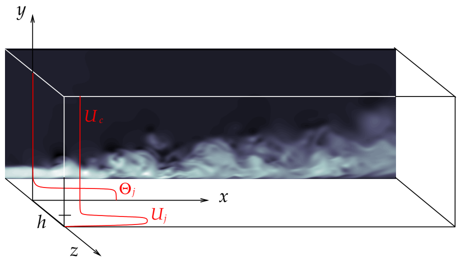

Figure 1. Schematic of the flow geometry.

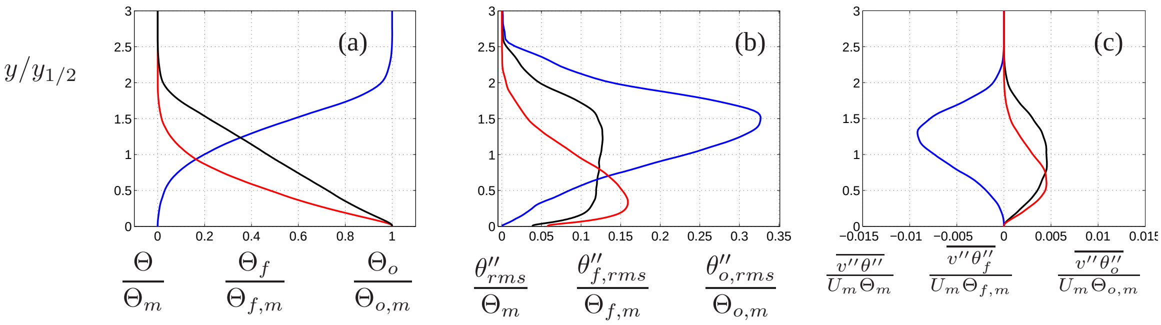

Figure 2. Statistics of oxidizer (blue), fuel (red) and passive (black) scalars at a downstream position of $x/h = 37$; Cross-stream profiles of (a) the mean scalars, (b) fluctuation intensity of the passive and reacting scalars, (c) wall-normal fluxes of scalars. Subscript m refers to the local maximum value of the corresponding variable.

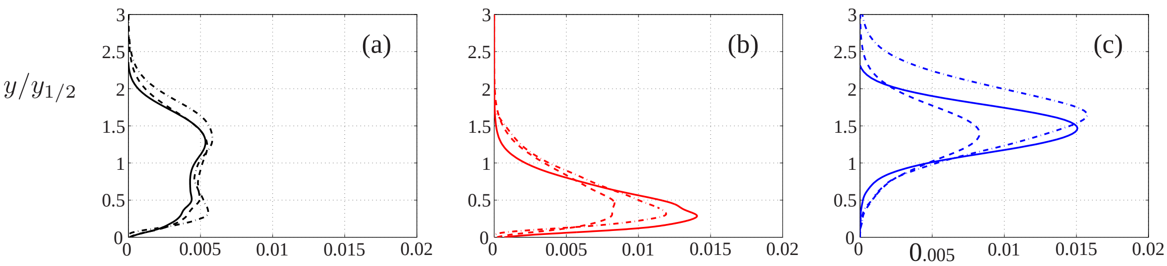

Figure 3. Cross-stream profiles of the SGS scalar variance Z_θ of (a) passive, (b) fuel and (c) oxidizer scalars at a downstream position of $x/h = 37$. Solid line: filtered DNS data, dashed line: DM (4) and dashed-dotted line: explicit algebraic model.

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