

## LES of two-phase flows with phase change using SGS models derived from DNS

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LES is conducted of a three-dimensional temporal mixing layer whose lower stream is initially laden with liquid drops which may evaporate during the simulation. The drops are much smaller than the Kolmogorov scale, which allows considering them as point sources for the flow. The gas-phase equations are written in an Eulerian frame for two perfect gas species (carrier gas and vapor emanating from the drops), while the liquid-phase equations are written in a Lagrangian frame. The effect of drop evaporation on the gas phase is considered through mass, momentum and energy source terms. The drop evolution is modeled using physical drops, or using computational drops to represent the physical drops. Simulations are performed using various LES models previously assessed on a DNS database. The LES equations were obtained from the DNS ones through spatial filtering; all terms in these LES equations were evaluated on the DNS database and those terms that were many orders of magnitude smaller than the leading terms were neglected. The models used in LES are for: (1) the SGS fluxes and (2) the filtered source terms (FST) based on computational drops. The LES, which are compared to filtered DNS results, were conducted with 64 times fewer grid points than the DNS, and up to 64 times fewer computational than physical drops. Several SGS models are evaluated by comparing the LES results with those of the filtered and coarsened DNS. It was found that both constant-coefficient Smagorinsky and dynamic Smagorinsky (SMD) SGS-flux models, though numerically stable, were overly dissipative and inhibited the generation of small-scale turbulent structures. The constant coefficient Gradient SGS-flux model, although more accurate, was not consistently stable over the range of mixing layer mass loadings, despite using DNS-calibrated coefficients; this deficiency was overcome by the dynamic Gradient (GRD) model, which performed like the constant-coefficient Scale Similarity model but, unlike it, did not require a priori calibration of the model coefficient. The FST model allowed up to a 32-fold reduction in computational drops compared to the number of physical drops without degradation of accuracy; a 64-fold reduction led to a slight decrease in accuracy.

Figures 1-6 illustrate examples of the comparison between DNS and LES. In all figures,  $x_1$  and  $x_2$  are the streamwise and the cross-stream coordinates of the mixing layer,  $\delta_{\omega,0}$  is the initial vorticity thickness of the layer,  $\rho_n$  is the drop number density (in  $\text{m}^{-3}$ ) and  $Y_v$  is the mass fraction of the evaporated fuel. All illustrations are contour plots in the same between-the-braid plane at the DNS transitional time for a simulation where the initial Reynolds number (based on the initial vorticity thickness) is 600, the initial drop mass loading is 20%, the initial carrier gas (air) temperature is 375K and that of the drops is 345K, with initially no-slip between drops and gas. Figures 1 and 2 represent the DNS results filtered and coarsened for comparison with the LES; in Fig. 1, only one out every 8 drops is shown, in order to compare with LES performed with computational drops. These LES results, with each computational drop representing 8 physical drops are depicted in Figs. 3 and 4 for the SMD model and Figs. 5 and 6 for the GRD model which are equivalent to plots in Figs. 1 and 2. Clearly, the SMD model is incapable of generating turbulence; this behavior is related to its overly dissipative aspect which was confirmed by examining velocity-fluctuation-based energy spectra. In contrast, the GRD model can replicate the filtered and coarsened DNS reasonably well. To appreciate the advantages of LES and particularly of the GRD model, consider the CPU times required for these simulations to reach the DNS transitional time: 2252 hours for DNS, and 37 hours for each of the LES, independent of the SGS model. The LES computational time decreases with decreasing number of computational drops: 21 hours (for both SMD and GRD) when a computational drop represents 16 physical drops, 14 hours (SMD) and 13 hours (GRD) when a computational drop represents 32 physical drops, and 10 hours (for both SMD and GRD) when a computational drop represents 64 physical drops.

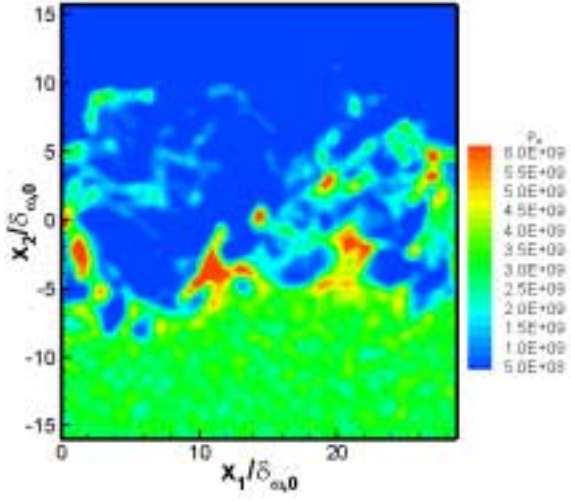


Fig. 1.

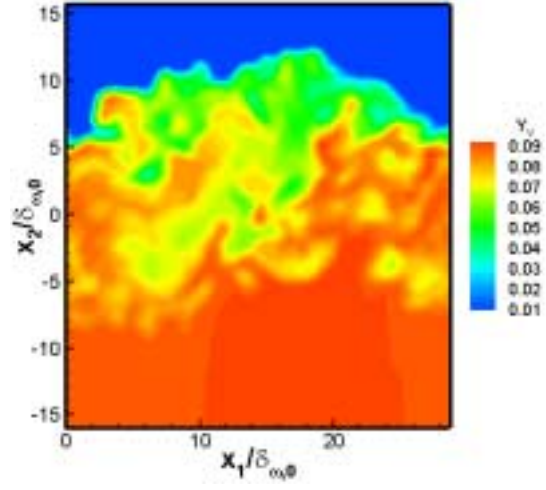


Fig. 2.

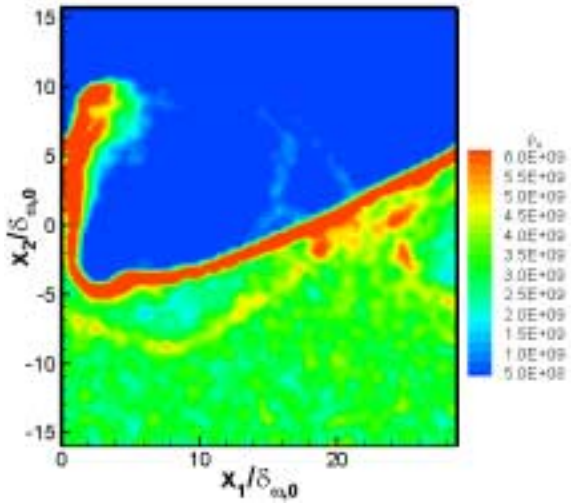


Fig. 3.

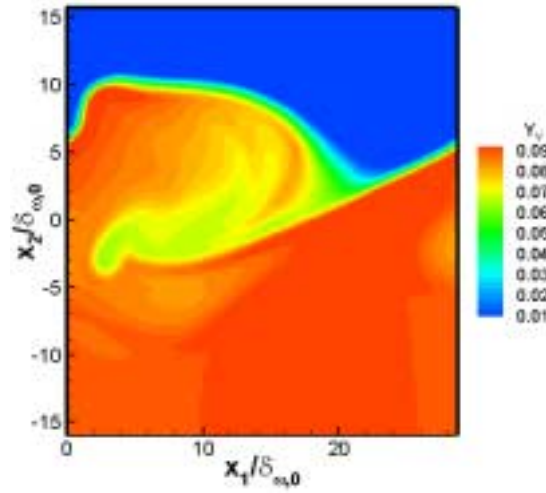


Fig. 4.

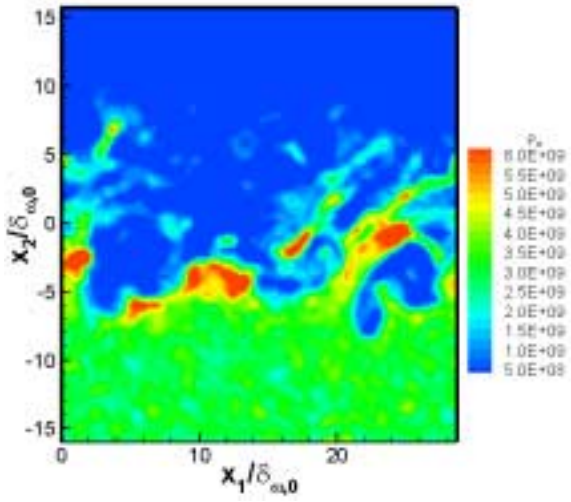


Fig. 5.

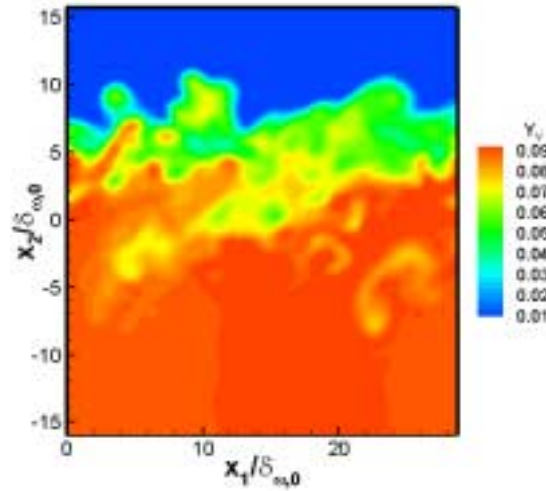


Fig. 6.