

Large Eddy Simulation of Turbulent Combustion via Filtered Mass Density Function

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The filtered mass density function (FMDF) methodology [1, 2] is employed as a subgrid scale (SGS) closure in large eddy simulation (LES) of various single-phase and two-phase turbulent reacting flows. The FMDF represents the joint probability density function of the SGS scalars, and is determined via the solution of its modeled transport equation. The accuracy of the method was previously established for single-phase 2-D, and 3-D temporally developing mixing layers and for a 2-D spatially developing planar jet by comparison with DNS data. In this work, we would like to further assess the applicability and the extent of validity of the FMDF method for SGS closure of both single-phase and two-phase turbulent combustion. This is conducted by implementation of the LES-FMDF for prediction of the physical and compositional structure of “high speed” turbulent methane and decane flames. The importance of chemical kinetics and SGS combustion models in such flames is well recognized. Two different approaches have been taken in the implementation of the chemistry: (i) a non-equilibrium model, and (ii) a near-equilibrium model. In (i), fuel oxidation is modeled via finite rate reduced mechanisms. In (ii), the flamelet library obtained from a laminar counterflow (opposed jet) flame configuration is used to characterize reaction. The library is constructed from the detailed oxidation mechanisms. The Sandia’s turbulent methane jet flames [3] are considered for partial validation of our computational models. The piloted jet flame configuration at Sandia Laboratory considers a momentum driven turbulent methane flame. Three basic flames considered, identified by Flames D, E, and F. The geometrical configurations in these flames is the same, but the jet inlet velocity is varied. In Flame D, the fuel jet velocity is the lowest and the flame is close to equilibrium with limited local flame extinction. The jet velocity increases from flames D to E to F, with noticeable non-equilibrium effects in the latter two. The droplet phase is simulated via a Lagrangian method with full mass, momentum and energy coupling between phases. The subgrid turbulence effects on droplet phase is modeled with an stochastic closure. LES of two-phase turbulent jets and dump combustors are conducted and the simulated results are compared with the available experimental data.

References

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- [3] Barlow, R. and Frank, J., Effects of Turbulence on Species Mass Fractions in Methane/Air Jet Flames, *International symposium on combustion*, **27**:1087–1095 (1998).