LARGE EDDY SIMULATION OF GRAVITATIONAL EFFECTS IN TRANSITIONAL AND TURBULENT GAS-JET DIFFUSION FLAMES

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INTRODUCTION

The influence of gravity on the spatial and the compositional structures of transitional and turbulent hydrocarbon diffusion flames are studied via large eddy simulation (LES) and direct numerical simulation (DNS) of round and planar jets. The subgrid-scale (SGS) closures in LES are based on the filtered mass density function (FMDF) methodology [1-3]. The FMDF represents the joint probability density function (PDF) of the SGS scalars, and is obtained by solving its transport equation. The fundamental advantage of LES/FMDF is that it accounts for the effects of chemical reaction and buoyancy exactly. The methodology is employed for capturing some of the fundamental influences of gravity in equilibrium flames via realistic chemical kinetic schemes. Some preliminary investigation of the gravity effects in non-equilibrium flames is also conducted, but with idealized chemical kinetics models.

APPROACH

The primary objective of this work is to develop and implement the LES/FMDF methodology for understanding of gravity effects in turbulent gas-jet diffusion flames. In addition, some DNS is also conducted for validation of some of our findings and for assessment of some of the modeling assumptions made in the LES procedure. In DNS, the coupled set of Navier-Stokes, energy, and scalar transport equations are solved together with the equation of state, a one-step kinetics model for the chemistry and constitutive relations for the molecular viscosity, diffusivity and conductivity. In LES/FMDF, the scalar field, $\boldsymbol{\phi} \equiv \phi_\alpha,\ \alpha = 1, 2, \ldots, N_s + 1$ (mass fractions and enthalpy) is obtained from the joint scalar FMDF [1],

$$F_L(\boldsymbol{\psi}, \mathbf{x}; , t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t)\zeta\left[\boldsymbol{\psi}, \boldsymbol{\phi}(\mathbf{x}', t)\right] H(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \tag{1}$$

where H denotes the filter function, and ζ is the "fine-grained" density [4]. The final form of the FMDF transport equation is

$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_i\rangle_L F_L]}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\langle\rho\rangle_\ell(\langle D\rangle_L + D_t)\frac{\partial(F_L/\langle\rho\rangle_\ell)}{\partial x_i}\right] + \frac{\partial}{\partial \psi_\alpha}\left[\Omega_m(\psi_\alpha - \langle\phi_\alpha\rangle_L)F_L\right] - \frac{\partial[\widehat{S}_\alpha F_L]}{\partial \psi_\alpha} \tag{2}$$

where, $\langle f(\mathbf{x}, t)\rangle_\ell$ and $\langle f(\mathbf{x}, t)\rangle_L = \langle\rho f\rangle_\ell/\langle\rho\rangle_\ell$ represent the filtered, and the Favre-filtered values of the transport variable $f(\mathbf{x}, t)$. In Eqs. (1) and (2), S_α, u_i, ρ, $\boldsymbol{\psi}$, and Ω_m, denote the production rate of species α, the ith component of the velocity vector, the density, the "composition space" of scalar $\boldsymbol{\phi}$, and the SGS mixing frequency, respectively. The molecular diffusivity coefficient, and the SGS diffusivity coefficient are denoted by D, and

D_t, respectively. The last term on the right hand-side (RHS) of Eq. (2) represents the effects of chemical reaction and is in a closed form. The first two terms on RHS represent the effects of SGS mixing and SGS convection, respectively and are closed via models similar to those used in conventional PDF methods [4].

Equation (2) is solved by the "Lagrangian Monte Carlo" procedure in which the FMDF is represented by an ensemble of computational elements. These elements are transported in the "physical space" by the combined actions of large scale convection and diffusion (molecular and subgrid). In addition, transport in the "composition space" occurs due to chemical reaction and SGS mixing. In doing so, the notional particles evolve via a "stochastic process," described by the set of stochastic differential equations (SDEs) [1]. These are coupled with the hydrodynamic solver which is via a "compact parameter" finite difference scheme.

Combustion is modeled via two chemistry models: (1) an equilibrium model via realistic kinetics, (2) a finite rate, single-step model for non-equilibrium flames. In (1), the LES/FMDF is employed in conjunction with equilibrium methane-oxidation model. This model is enacted via "flamelet" simulations; which consider a laminar counterflow (opposed jet) flame configuration. The full methane oxidation mechanism of the Gas Research Institute (GRI) accounting for 53 species and 325 elementary reactions is employed. At low strain rates, the flame is close to equilibrium. Thus, the thermo-chemical variables are determined completely by the "mixture fraction." This flamelet library is coupled with our LES/FMDF solver in which transport of the mixture fraction is considered. In (2), methane oxidation is modeled via a finite-rate, single-step global kinetics model.

RESULTS AND DISCUSSIONS

The (few) sample results presented in this section pertain only to the effects of gravity on the overall flow structure in gas jet diffusion flames. LES is conducted of three-dimensional (3D) round jet flames involving methane combustion under zero- and normal-gravity conditions. In the latter, the gravity vector is aligned opposite to the direction of the axial jet flow. The effect of gravity on the evolution of the jet flame is shown in Fig. 1, where the contour plots of the instantaneous filtered values of CO_2 mass fraction are considered. As expected, the flow is initially 2D (axisymmetric), and then becomes strongly 3D with significant small scales. In the absence of gravity, turbulence levels decrease due to damping of flow instabilities by exothermicity. In the presence of gravity, however, the buoyancy induced instabilities lead to increased turbulence, particularly at small scales. The combustion generated density variations and buoyancy induced instabilities lead to deformation of large-scale organized structures. This is known as "flickering" [5] and results in increase of hydrodynamic mixing.

The enhanced mixing discussed above does not always yield increased combustion. Analysis of the compositional structure of the non-equilibrium flame in zero- and normal-gravity indicates that in the absence of gravity, the peak temperature is close to adiabatic and the rate of reactant conversion is significant. However, in the presence of gravity the flame experiences local extinction due to large straining caused by enhanced small scale structures.

Some of the physical features captured by LES/FMDF are verified by DNS of 3D planar jet

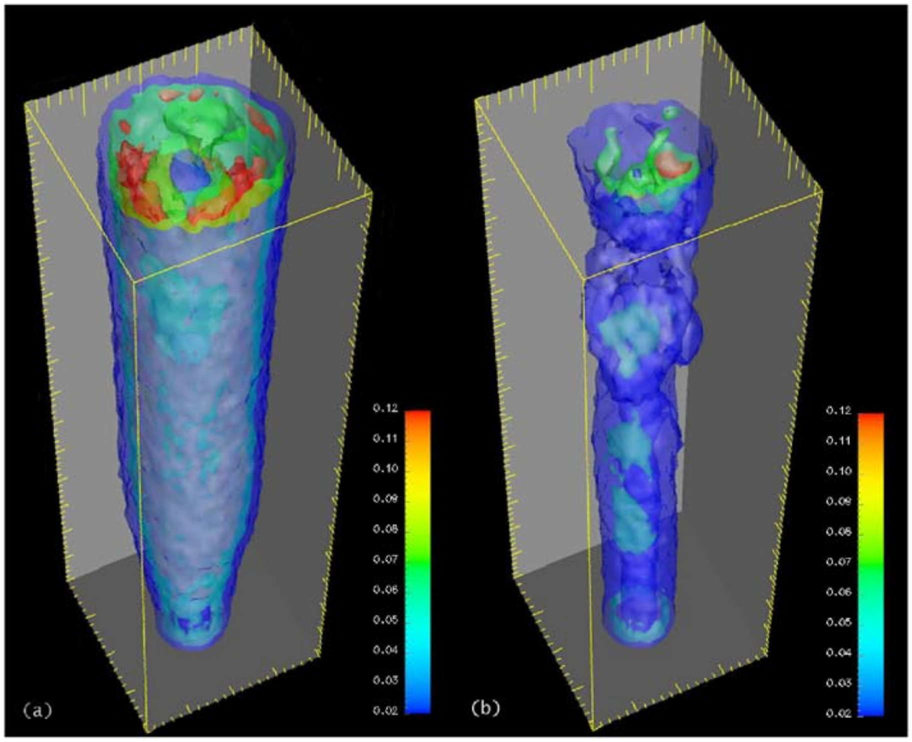

Figure 1: Contour plots of the instantaneous, filtered values of the mass fraction of CO_2 in an upward methane round jet flame under non-equilibrium condition, as predicted by LES-FMDF. (a) Zero gravity, (b) Normal gravity.

flames. These simulations are based on an idealized single-step irreversible chemical kinetics model in which the range of parameters such as the Reynolds and Damkohler number are smaller than those considered in LES. Obviously, a quantitative comparison between DNS and LES results is not possible. Figure 2 shows the contour plots of the vorticity. Similar to that captured by LES, the flow is initially dominated by large scale 2D vortical structures and then becomes strongly 3D with significant small scales. The effect of reaction is consistent with that obtained by LES as discussed above. All of the LES and DNS results are analyzed statistically. These will be presented at the workshop. In all cases, it is observed that gravity enhances turbulence, and thus promotes mixing. In some cases, this enhanced mixing leads to a larger rate of reactant conversion. This is always true in equilibrium flames, but not always true in non-equilibrium flames. In the latter, the enhanced strain field may yield local flame extinction and reduction in reactant conversion.

WORK IN PROGRESS

Our current work is focused on analysis of non-equilibrium diffusion flames with realistic chemical kinetics. In future work, we plan to develop and implement the joint velocity-scalar FMDF methodology for LES of diffusion flames. This would have the advantage of closing the effects of SGS convection [6].

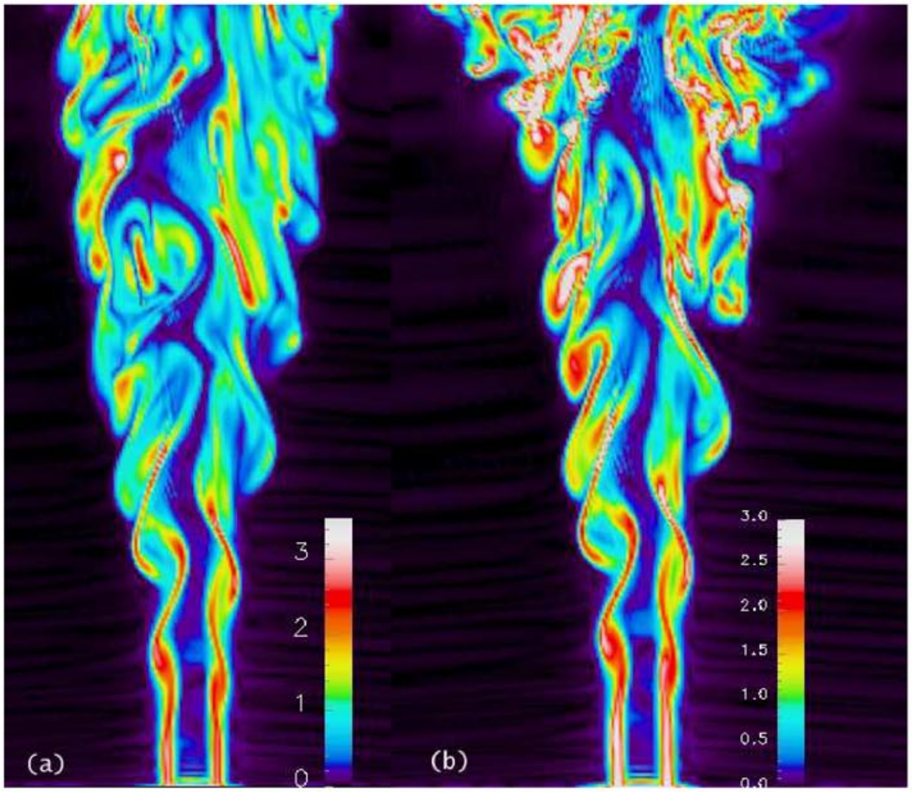

Figure 2: Contour plots of the instantaneous vorticity magnitude in an upward reacting, 3D planar jet flame as obtained by DNS. (a) Zero gravity, (b) Normal gravity.

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