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

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## OBJECTIVE

The basic objective of this work is to assess the influence of gravity on "the compositional and the spatial structures" of transitional and turbulent diffusion flames via large eddy simulation (LES), and direct numerical simulation (DNS). The DNS is conducted for appraisal of the various closures employed in LES, and to study the effect of buoyancy on the small scale flow features. The LES is based on our "filtered mass density function" (FMDF) model [1]. The novelty of the methodology is that it allows for reliable simulations with inclusion of "realistic physics." It also allows for detailed analysis of the unsteady large scale flow evolution and compositional flame structure which is not usually possible via Reynolds averaged simulations.

## FORMULATION

The flow field under investigation is that of a jet-flame in which a high speed fuel is injected into a low speed or stagnant coflowing stream of oxidizer. This flow is inherently time-dependent and three-dimensional (3D). Nevertheless, some 2D (planar) simulations (via both LES and DNS) are also conducted for validation of the numerical methods and for determining the range of parameters. We have primarily considered methane/air combustion because of the rich extent of literature on methane oxidation mechanism, and availability of significant data in such flames. The application of a spatially & temporally invariant and localized filter function to the fundamental transport equations of reacting flows yields:

$$\frac{\partial \langle \rho \rangle_\ell}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = -\frac{\partial \langle p \rangle_\ell}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle_\ell}{\partial x_i} - \frac{\partial \mathcal{T}_{ij}}{\partial x_i} + \langle \rho \rangle_\ell \, g_j \tag{2}$$

$$\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial \langle J_i^\alpha \rangle_\ell}{\partial x_i} - \frac{\partial \mathcal{M}_i^\alpha}{\partial x_i} + \langle \rho S_\alpha \rangle_\ell, \quad \alpha = 1, 2, \ldots, \sigma \tag{3}$$

where filtered and Favre-filtered values of the transport variable $f(\mathbf{x}, t)$ are represented by $\langle f \rangle_\ell$ and $\langle f \rangle_L = \langle \rho f \rangle_\ell / \langle \rho \rangle_\ell$, respectively. In these equations $u_i$ and $\rho$ are the velocity vector and the density, $p$ denotes the pressure, $g_j$ denotes the gravity vector, and $\tau_{ij}$, $J_i^\alpha$ are the molecular viscosity tensor and diffusivity vector, respectively. The scalars include mass fraction of chemical species, $\phi_\alpha \equiv Y_\alpha$, $\alpha = 1, 2, \ldots, N_s$, and specific enthalpy, $\phi_\sigma \equiv h = \sum_{\alpha=1}^{N_s} h_\alpha \phi_\alpha$, in which $h_\alpha = h_\alpha^0 + \int_{T_0}^T c_{p_\alpha}(T') dT'$ ($T$ is the temperature). These equations are

closed by the constitutive relations. The hydrodynamic subgrid scale (SGS) closure problem is associated with $\mathcal{T}_{ij} = \langle\rho\rangle_\ell(\langle u_i u_j\rangle_L - \langle u_i\rangle_L\langle u_j\rangle_L)$ and $\mathcal{M}_i^\alpha = \langle\rho\rangle_\ell(\langle u_i\phi_\alpha\rangle_L - \langle u_i\rangle_L\langle\phi_\alpha\rangle_L)$ denoting the SGS stresses and the SGS scalar fluxes, respectively. The term $\langle\rho S_\alpha\rangle_\ell = \langle\rho\rangle_\ell\langle S_\alpha\rangle_L$ $(\alpha = 1, 2, \ldots, N_s)$ denoting the filtered reaction rates. The joint velocity-scalar FMDF is formally defined as:

$$\mathcal{F}_L(\mathbf{V}, \psi, \mathbf{x}; t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t)\xi[\mathbf{V}, \mathbf{U}(\mathbf{x}', t), \psi, \phi(\mathbf{x}', t)] H(\mathbf{x}' - \mathbf{x})d\mathbf{x}' \tag{4}$$

where $H$ is the filter function, $\psi$ denotes the composition domain of the scalar array, $\phi(\mathbf{x}, t)$, and $\mathbf{V}$ denotes the probability domain of the random velocity vector, $\mathbf{U}(\mathbf{x}, t)$. The term $\xi[\mathbf{V}, \mathbf{U}(\mathbf{x}, t), \psi, \phi(\mathbf{x}, t)]$ is the fine-grained velocity-scalar density. Equation (4) implies that the FMDF is the *mass weighted spatially filtered* value of the fine-grained density. Starting from the original (unfiltered) transport equations of the velocity and the scalar variables, one may derive the transport equation for the joint velocity-scalar FMDF. By integrating the resulting equation over the velocity space, the transport equation for the joint filtered mass density function of the scalars, $F_L$ is obtained:

$$\frac{\partial F_L}{\partial t} + \frac{\partial\langle u_i\rangle_L F_L}{\partial x_i} = -\frac{\partial[\langle u_i|\psi\rangle_\ell - \langle u_i\rangle_L]F_L}{\partial x_i} + \frac{\partial}{\partial x_i}\left\langle\rho D\frac{\partial\zeta}{\partial x_i}\right\rangle_\ell - \frac{\partial[\hat{S}_\alpha(\psi)F_L]}{\partial\psi_\alpha}$$

$$-\frac{\partial^2}{\partial\psi_\alpha\partial\psi_\beta}\left[\left\langle\rho D\frac{\partial\phi_\alpha}{\partial x_i}\frac{\partial\phi_\beta}{\partial x_i}|\psi\right\rangle_\ell F_L/\hat{\rho}\right] \tag{5}$$

where $\zeta$ represents the scalar fine-grained density, $D$ is the molecular diffusion coefficient, $\langle\mathcal{A}|\mathcal{B}\rangle_\ell$ denotes the filtered value of the variable $\mathcal{A}$, "conditioned" on $\mathcal{B}$, and the hat is used to emphasize the quantities which are dependent only on the scalar field. It is noted that in this "exact" transport equation the terms associated with and chemical reaction is represented in a closed form.

## PROGRESS TO DATE

Up to now, we have conducted several DNS and LES of 2D and 3D jet flames. Most of the LES are conducted via the scalar FMDF methodology; the use of the joint velocity-scalar FMDF is the subject of our ongoing investigation (please see next section). The SGS mixing term in this equation is modeled via the IEM closure as discussed in Ref. [1]. The finite-rate chemistry effects are explicitly included in this way since the chemistry is closed in the formulation. Numerical solution of the scalar FMDF is obtained with a hybrid Eulerian/Lagrangian scheme. The hydrodynamic field is obtained by solving the filtered continuity and momentum equations with a compact parameter finite-difference scheme. The scalar quantities include mass fraction of chemical species and enthalpy. The FMDF is represented by an ensemble of Lagrangian Monte Carlo [2] particles which are freely transported in the physical space by the combined actions of large scale convection and diffusion (molecular and subgrid). Transport in the composition space occurs due to chemical reaction and SGS mixing. Thus, the grid-free Lagrangian procedure considers "notional particles" whose evolution can be computed via a "stochastic process" to simulate motion in

physical space by convection and diffusion. The compositional values of particles are changed due to mixing and reaction. These are represented by the stochastic differential equations. The oxidation of methane is simulated via a one-step global mechanism [3].

The examination of the physical flame structure indicates that both the large and the small flow scales are significantly influenced by buoyancy. Expectedly, in cases with large values of the Froude number combustion has found to damp the jet growth due to adverse effects of chemical heat release on the growth of hydrodynamic instabilities. However, in cases with relatively low values of the Froude number, the combustion-generated density variations result in buoyancy induced instabilities and rapid jet growth (as compared to the non-reacting jet). This results in significant enhancement of turbulence at large and small scales, thus yields an increase in mixing and combustion. These results are consistent with experimental results on normal and microgravity jet flames [4], and suggest that there is a strong two-way coupling between turbulence and combustion in nonpremixed normal gravity jet flames which is very different from that in microgravity. These results also suggest that the models which are developed and tested at normal gravity flames may not work properly in microgravity, and vice versa. Our results also indicate that LES/FMDF is able to capture the large scale features of turbulence correctly. The effect of the buoyancy on the small scale flow quantities such as the SGS stresses and the closures used for these quantities needs to be studied further. Our preliminary results indicate that the magnitude of the SGS stresses, the SGS scalar fluxes and the SGS unmixedness enhance by the gravity.

Our investigation of the effects of gravity on the compositional structure of microgravity and normal gravity jet flames indicate that the gravity modifies significantly this structure. The finite rate chemistry effects, as portrayed by the scatter plots of the temperature in the mixture fraction space, are more significant in microgravity flame than those in normal grav- ity. This is attributed to the fact that mixing and combustion are intensified by buoyancy in normal gravity, and suggests that the ignition/extinction characteristics of the transi- tional/turbulent flames are dependent on the gravity at least at low to moderate values of the Froude number. An examination of the compositional flame structure for various flames also indicates that the gravity modifies the distribution of strain field, the major species in the flame zone, and the flame thickness.

The LES/FMDF predictions compare favorably with DNS data provided that the mixing frequency coefficient in the SGS mixing (IEM) model is assigned properly. This coefficient is somewhat dependent on the gravity level. The reason for this dependence is that the flow is not fully turbulent, specially near the inlet. Nevertheless, the values of the SGS scalar dissipation predicted by the model correlates very well with those obtained via DNS at all gravity levels. The large and the small scale flow structures are significantly modified by the gravity, resulting in variation in model coefficient at transitional jet region. In addition to DNS and LES/FMDF, we also simulated the jet flames via a conventional LES in which the SGS scalar correlations are ignored (this is labeled as LES-FD). A comparison between DNS and LES-FD indicates that in both zero- and normal-gravity environment the SGS scalar correlations have a strong influence on the large scale flow quantities; so if they are neglected the results would be erroneous.

## WORK IN PROGRESS

Work is also in progress on the following issues which are of interest to this project:

(1) We are considering the 12-step reduced kinetics mechanism of methane-air oxidation [5] in conjunction with the ISAT routine [6] in our scalar LES/FMDF. If this scheme proves to be computationally feasible, we will utilize it in our future simulations.

(2) Under another project, we have recently developed a methodology, termed the velocity filtered density function (VFDF) which accounts for the PDF of the SGS velocity vector. At this point, the formulation is valid for constant density turbulent flow. We are currently extending the methodology to account for the joint PDF of the SGS velocity and scalars. If the outcome of this work is successful, the joint velocity-scalar FMDF will be constructed and will be used for the jet flame simulation.

(3) We are conducting a feasibility assessment of a new computational methodology, termed the "Spectral/hp Element" method [7]. The advantage of this methodology is that it contains spectral accuracy and it also allows for utilization of "unstructured" grids. This assessment is being done for possible replacement of our current CFD mean flow solver with this methodology so that we can consider a larger computational domain for our jet flame LES and DNS.

## ACKNOWLEDGMENT

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